



FIG. 1

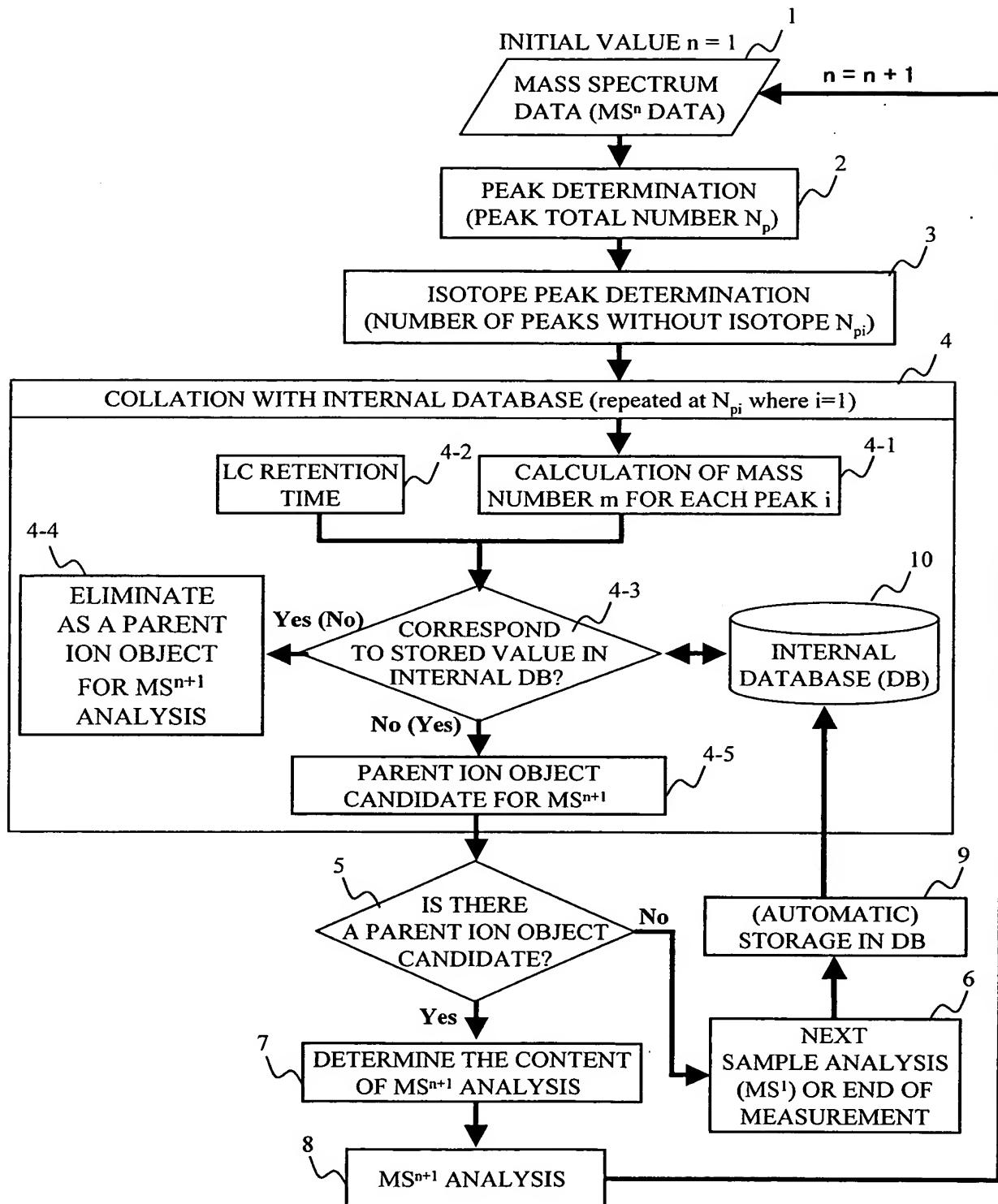


FIG. 2

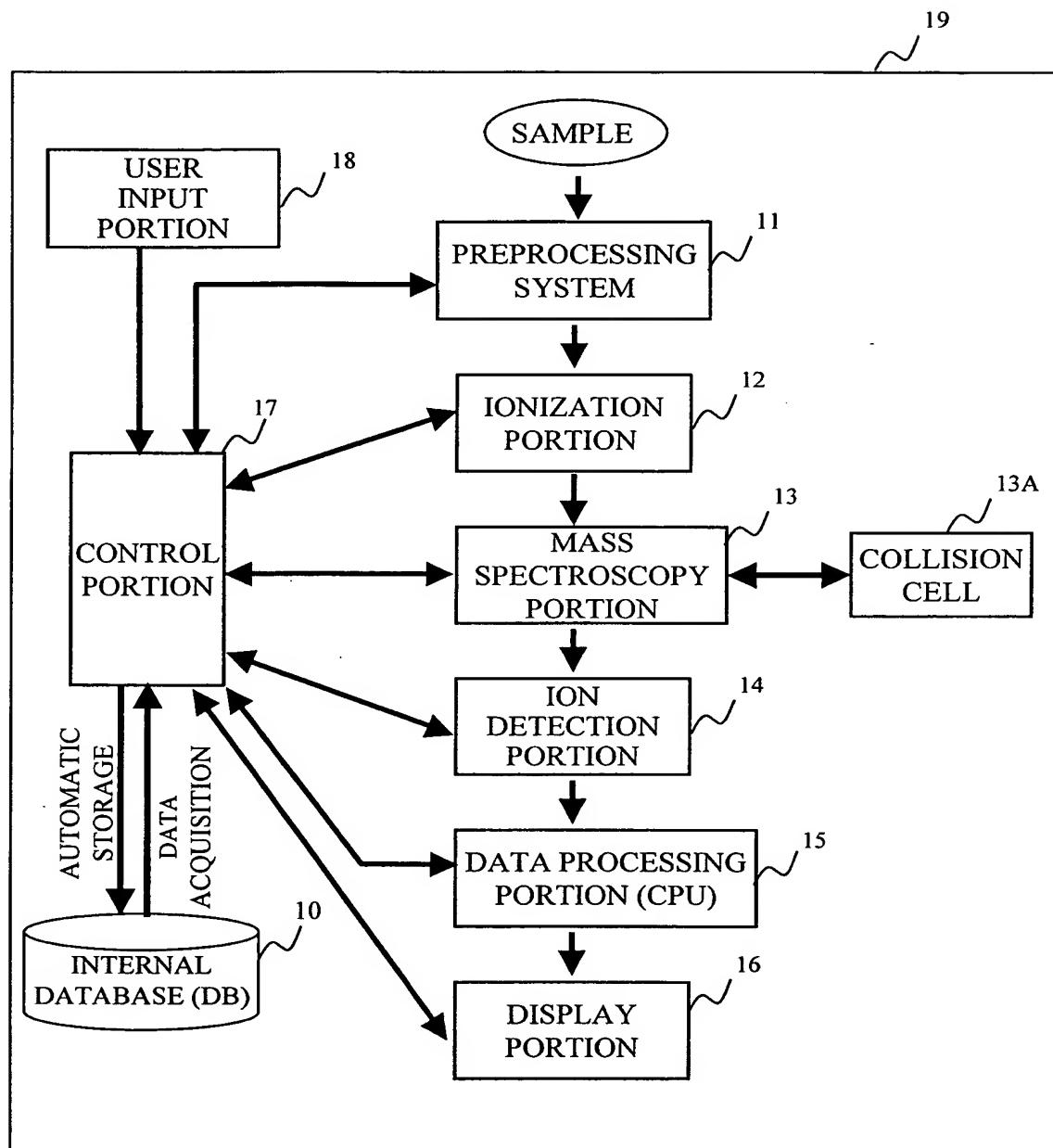


FIG. 3 A

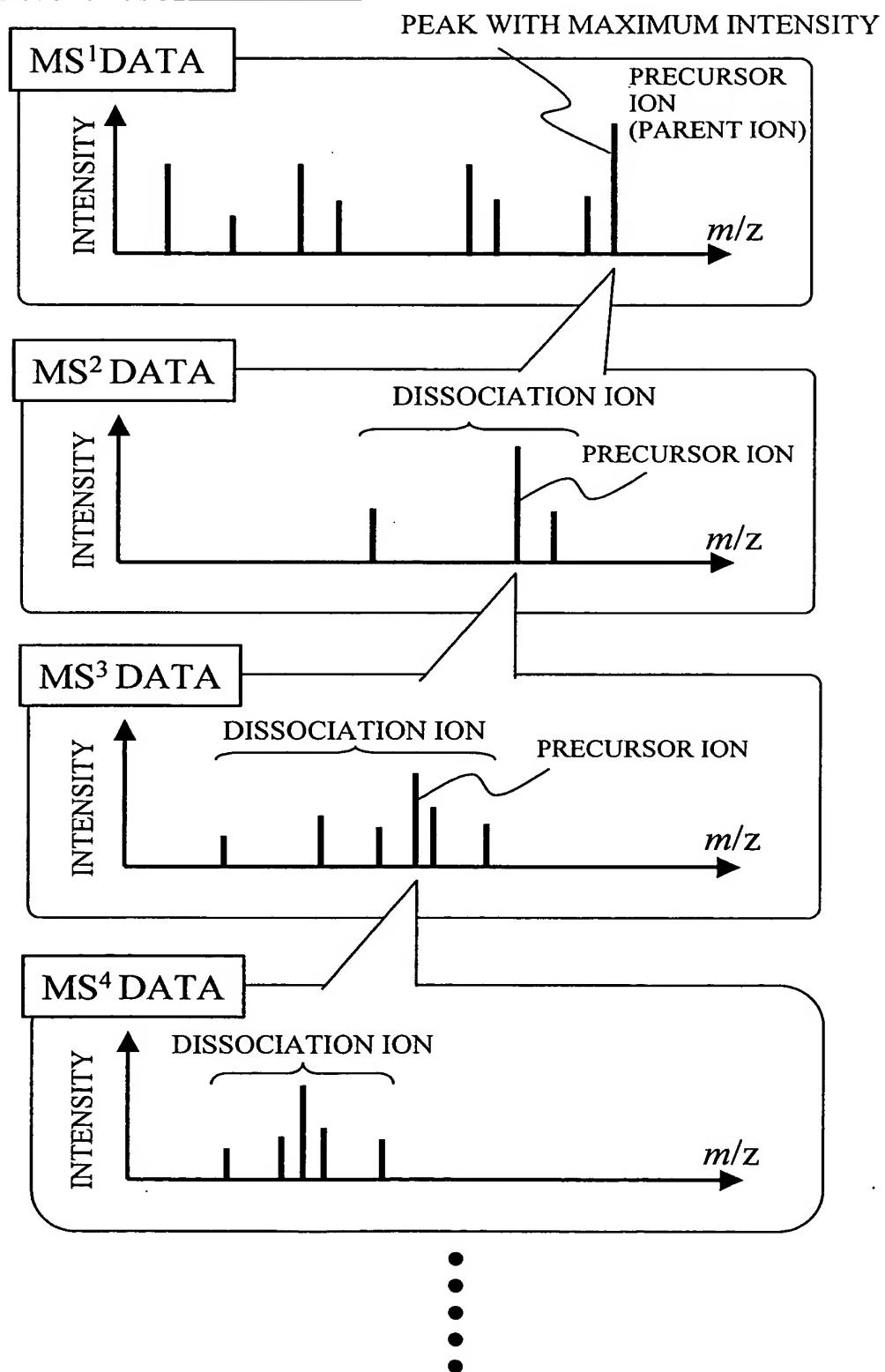
PRIOR ART METHOD

FIG. 3 B

EMBODIMENT 1

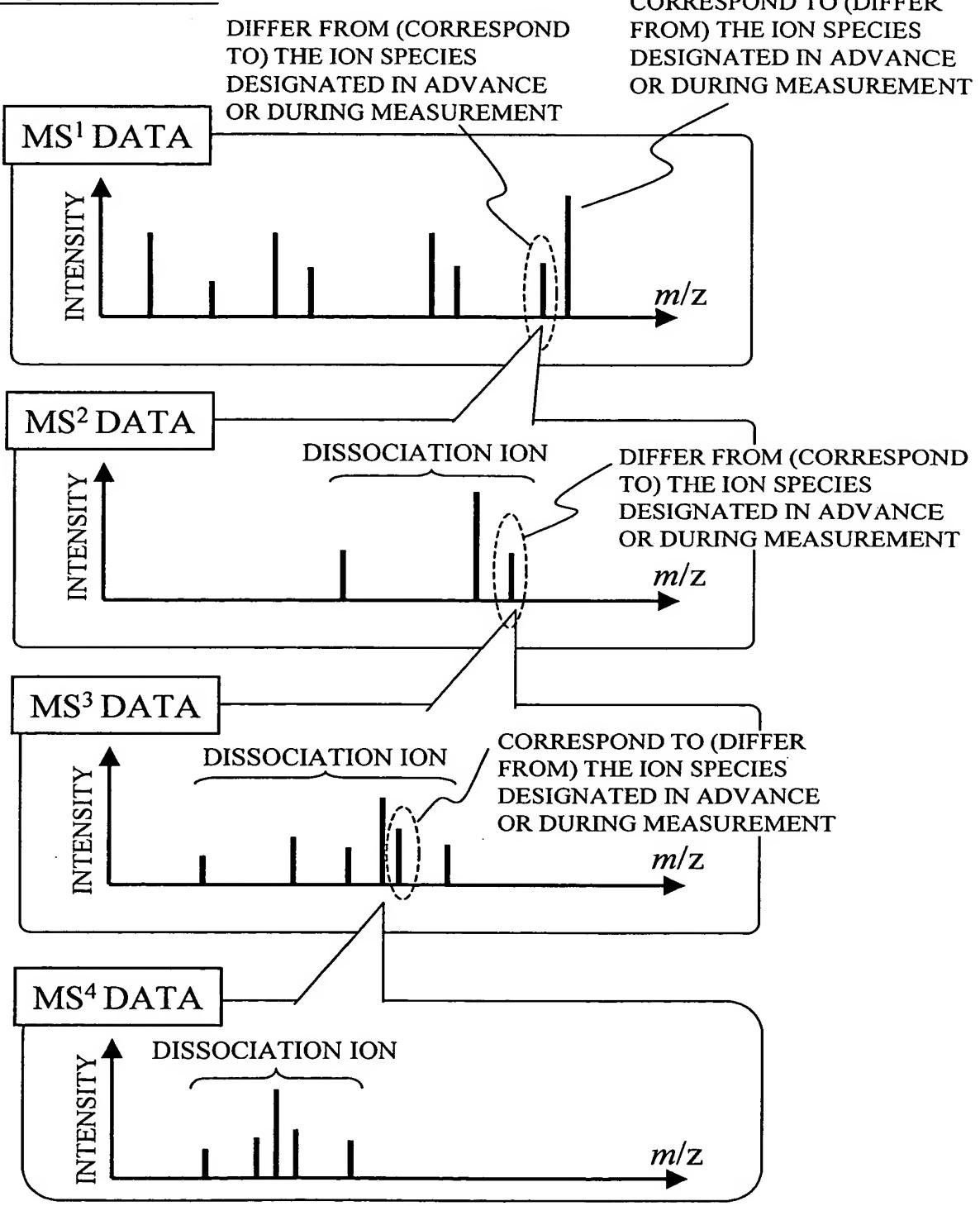


FIG. 3 C

EMBODIMENT 2

DIFFER FROM (CORRESPOND
TO) THE ION SPECIES
DESIGNATED IN ADVANCE OR
DURING MEASUREMENT

CORRESPOND TO (DIFFER FROM) THE ION SPECIES DESIGNATED IN ADVANCE OR DURING MEASUREMENT

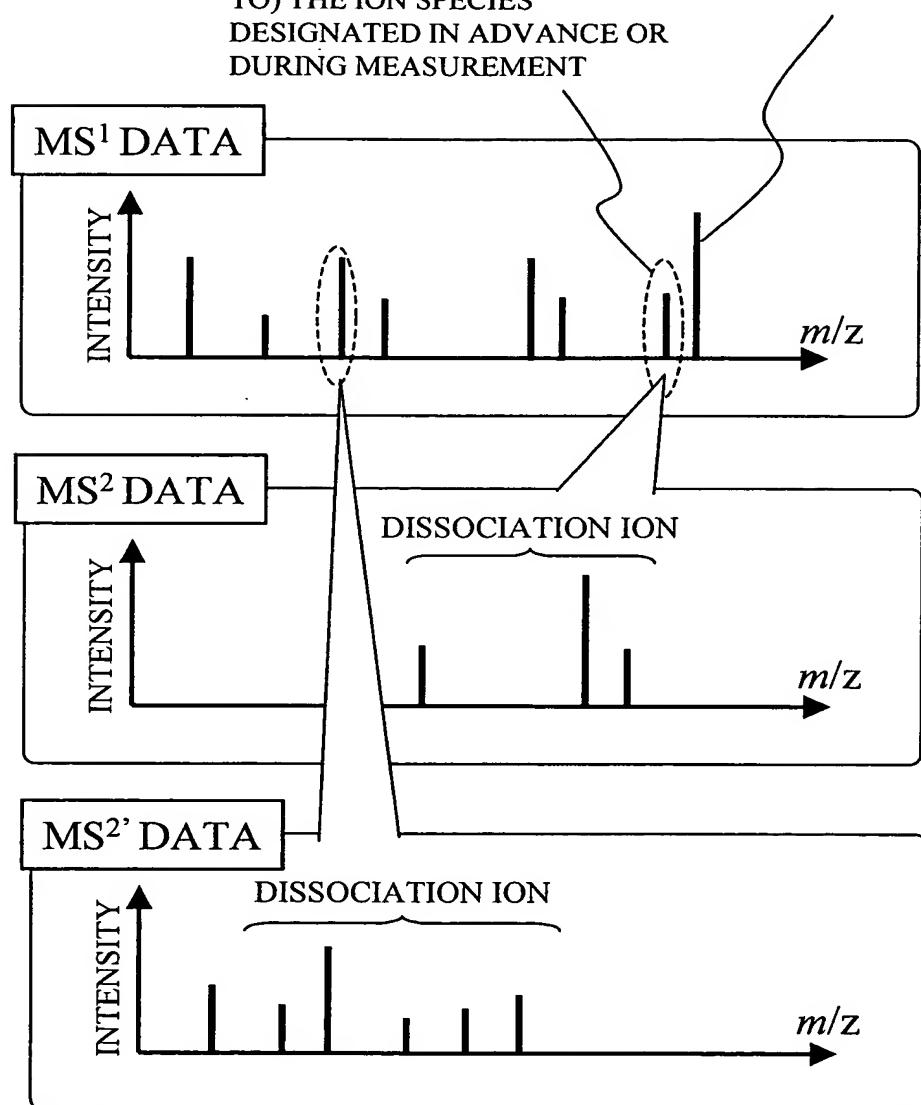


FIG. 4

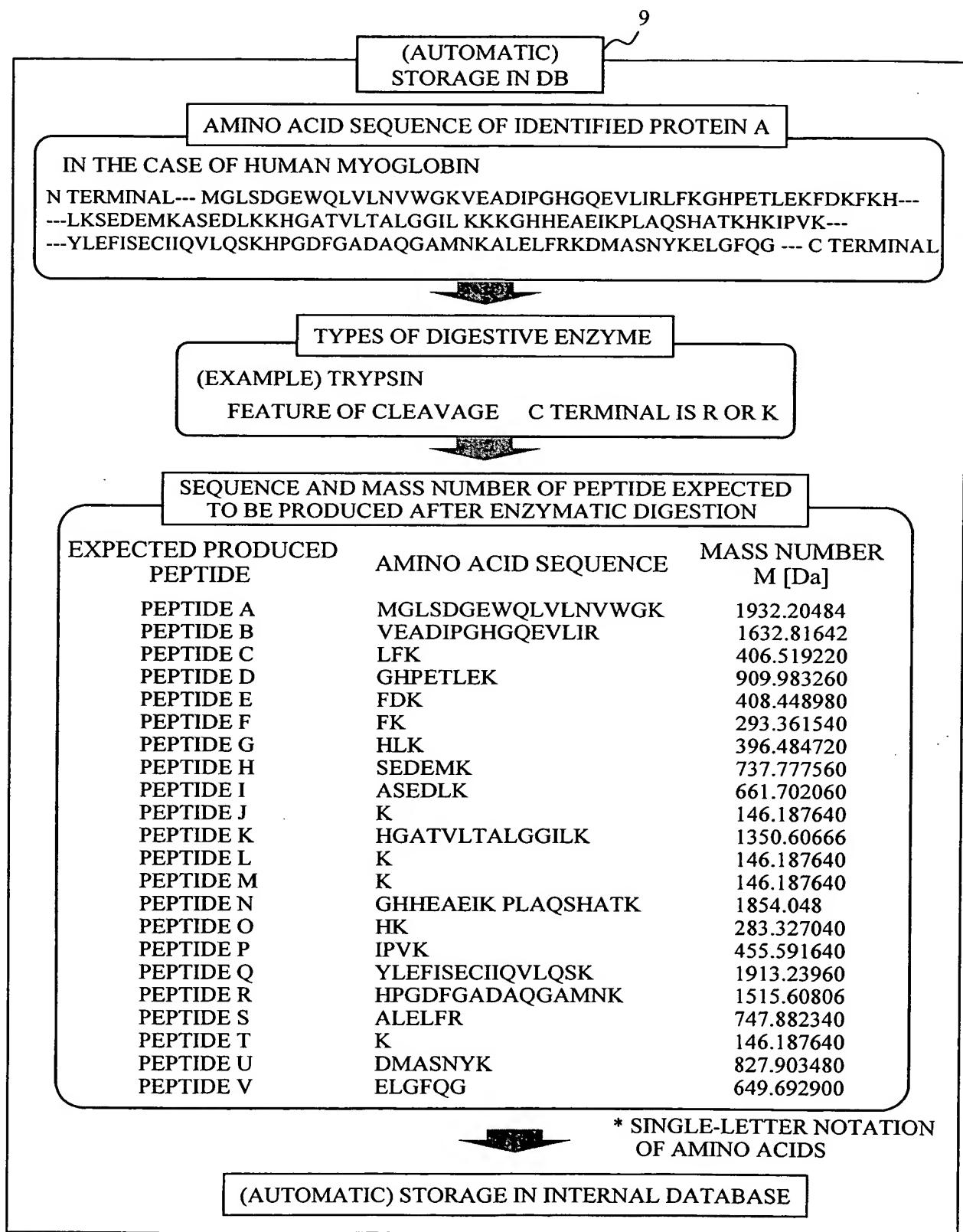
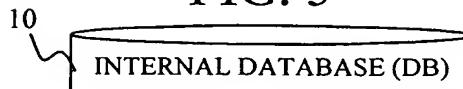


FIG. 5



CONTENT OF THE INTERNAL DATABASE

- CHARACTERISTICS DATA OF A PEPTIDE THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
 (MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

PEPTIDE NAME /SEQUENCE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
PEPTIDE A	200	1	200	15160	20	2
PEPTIDE B	700	2	350	2100	28	3
PEPTIDE C	450	1	450	4754	35	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A PEPTIDE DERIVED FROM A PROTEIN THAT HAS ONCE BEEN IDENTIFIED OR THAT SHOULD BE ELIMINATED FROM THE OBJECTS FOR TANDEM ANALYSIS
 (PROTEIN NUMBER, ID NUMBER, MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

PEPTIDE NAME /SEQUENCE	PROTEIN NAME	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
PEPTIDE A	PROTEIN A	570	1	570	25010	25	2
PEPTIDE B	PROTEIN A	652	1	652	3140	32	3
PEPTIDE C	PROTEIN A	652	2	326	58754	45	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
PEPTIDE D	PROTEIN B	1042	2	521	6456	22	2
PEPTIDE E	PROTEIN B	718	2	359	3080	35	3
PEPTIDE F	PROTEIN B	671	2	335.5	8054	48	3
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A SUGAR CHAIN THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
 (MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

SUGAR CHAIN NAME /STRUCTURE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
SUGAR CHAIN A	1002	2	501	15710	55	2
SUGAR CHAIN B	840	2	420	8340	34	3
SUGAR CHAIN C	1280	2	640	10754	42	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF A CHEMICAL SUBSTANCE THAT HAS ONCE BEEN SUBJECTED TO MSⁿ (n ≥ 2) MEASUREMENT
 (MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

CHEMICAL SUBSTANCE NAME/STRUCTURE	m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
CHEMICAL SUBSTANCE A	270	1	270	85510	23	2
CHEMICAL SUBSTANCE B	358	1	358	9840	47	2
CHEMICAL SUBSTANCE C	682	2	341	20764	82	2
⋮	⋮	⋮	⋮	⋮	⋮	⋮

- CHARACTERISTICS DATA OF AN ION SPECIES DERIVED FROM NOISE OR IMPURITIES
 (MASS NUMBER m, RETENTION TIME IN LC τ, VALENCE z, MASS-TO-CHARGE RATIO m/z, DETECTION INTENSITY I, ANALYSIS CONDITION)

m [Da]	z [-]	m/z	I	τ [min]	ANALYSIS CONDITION (EXAMPLE: ORDER OF TANDEM ANALYSIS)
361	1	361	-	15	-
640	1	640	-	40	-
740	1	740	-	31	-
⋮	⋮	⋮	⋮	⋮	⋮

FIG. 6

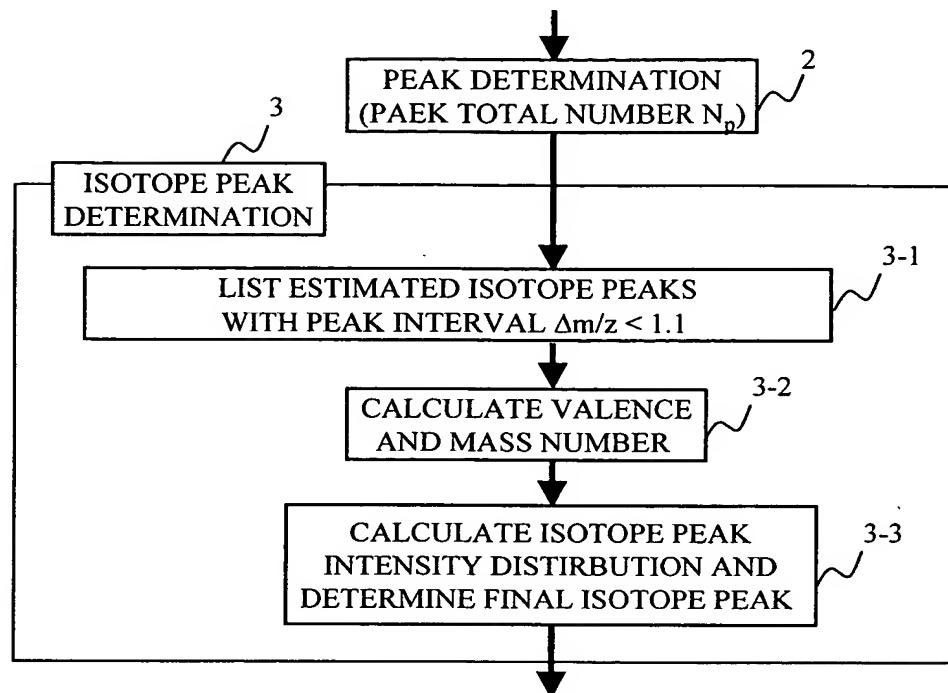


FIG. 7

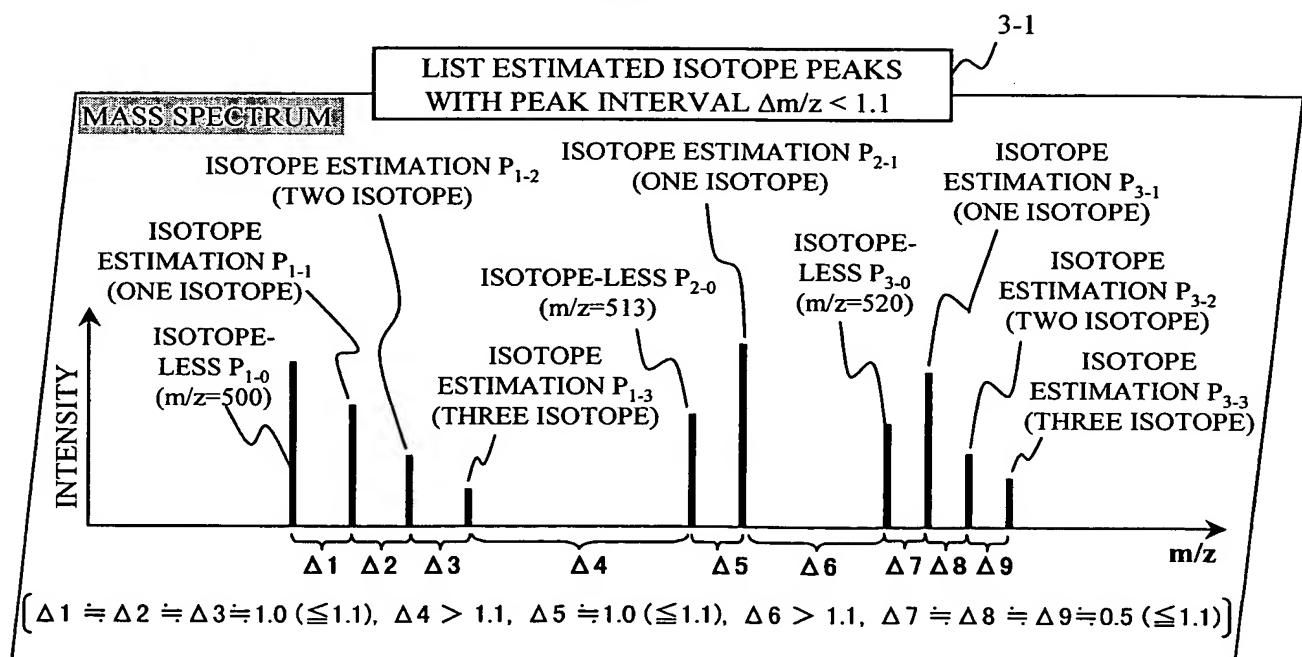


FIG. 8

3-2

CALCULATION OF VALENCE AND MASS NUMBER

(m_H : MASS NUMBER OF PROTON)

ISOTOPE-LESS PEAK P₁₋₀
 PEAK WITH ONE ISOTOPE P₁₋₁ > Δ₁
 PEAK WITH TWO ISOTOPE P₁₋₂ > Δ₂
 PEAK WITH THREE ISOTOPE P₁₋₃ > Δ₃ → { Δ₁ = Δ₂ = Δ₃ = 1.0 = Δ(C¹³-C¹²)/z = 1.0/z ⇒
 VALENCE z=1
 MASS NUMBER m_{p1} OF P₁₋₀ IS
 499 FROM m/z=500 = (m_{p1} + m_H × z)/z

ISOTOPE-LESS PEAK P₂₋₀
 PEAK WITH ONE ISOTOPE P₂₋₁ > Δ₅ → { Δ₅ = 1.0 = Δ(C¹³-C¹²)/z = 1.0/z ⇒
 VALENCE z=1
 MASS NUMBER m_{p2} OF P₂₋₀ IS
 512 FROM m/z=513 = (m_{p1} + m_H × z)/z

ISOTOPE-LESS PEAK P₃₋₀
 PEAK WITH ONE ISOTOPE P₃₋₁ > Δ₇
 PEAK WITH TWO ISOTOPE P₃₋₂ > Δ₈
 PEAK WITH THREE ISOTOPE P₃₋₃ > Δ₉ → { Δ₇ = Δ₈ = Δ₉ = 0.5 = Δ(C¹³-C¹²)/z = 1.0/z ⇒
 VALENCE z=2
 MASS NUMBER m_{p3} OF P₃₋₀ IS
 1038 FROM m/z=520 = (m_{p3} + m_H × z)/z

FIG. 9 A

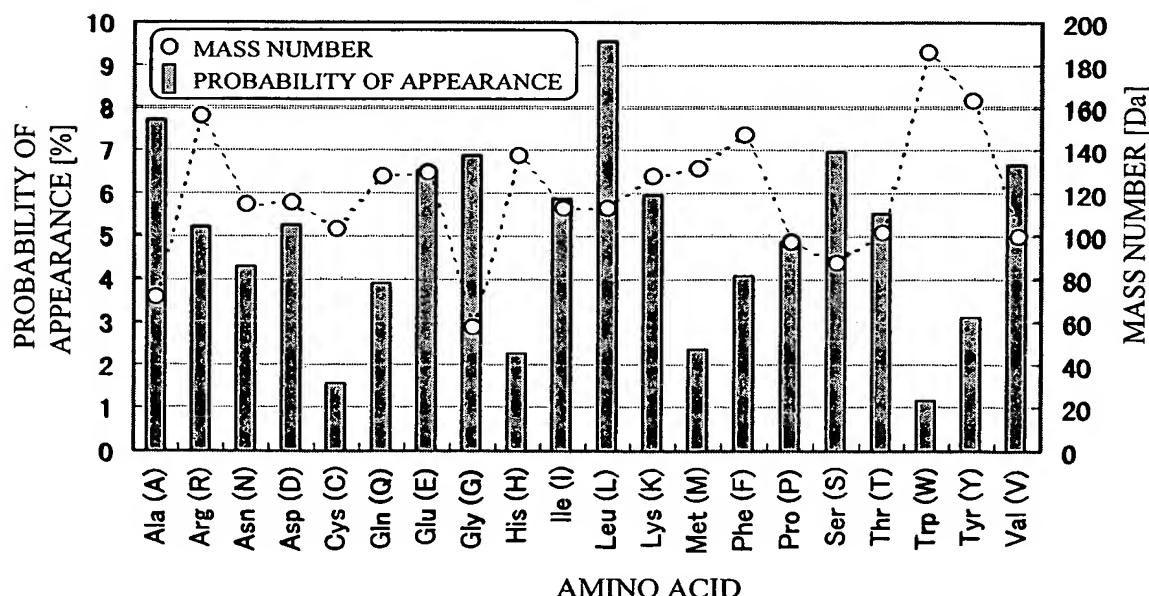


FIG. 9 B

3-3

CALCULATION OF ISOTOPE PEAK INTENSITY DISTRIBUTION AND DETERMINATION OF FINAL ISOTOPE PEAK

CALCULATION OF EACH ELEMENT NUMBER FROM MASS NUMBER

IN THE CASE OF A PEPTIDE ($C_{Nc}N_{Nn}H_{Nh}O_{No}S_{Ns}$)

$$\left\{ \begin{array}{l} \text{NUMBER OF C: } Nc = m \times nC / 111.1807 \\ \text{NUMBER OF O: } No = m \times nO / 111.1807 \\ \text{NUMBER OF N: } Nn = m \times nN / 111.1807 \\ \text{NUMBER OF H: } Nh = m \times nH / 111.1807 \\ \text{NUMBER OF S: } Ns = m \times nS / 111.1807 \end{array} \right.$$

TABLE A: EACH ELEMENT NUMBER PER AVERAGE AMINO ACID

nC	nO	nN	nH	nS
4.9583	1.4733	1.3547	7.8185	0.0396

CALCULATION OF ISOTOPE PEAK INTENSITY DISTRIBUTION

IN THE CASE WHERE ONLY AN ISOTOPE (C^{13}) IS CONSIDEREDISOTOPE PEAK INTENSITY P_{Nis} (WHEN NUMBER OF ISOTOPES IS Nis):

$$P_{Nis} = [Nc C_{Nis} \cdot pC(1)^{(Nc-Nis)} \cdot pC(2)^{Nis}] \times pH(1)^{Nh} \cdot pN(1)^{Nn} \cdot pO(1)^{No} \cdot pS(1)^{Ns}$$

TABLE B: MASS NUMBER AND ABUNDANCE RATIO OF EACH ISOTOPE ELEMENT

	MASS NUMBER	ABUNDANCE RATIO
C	$mC(1)$ 12	$pC(1)$ 0.9889
	$mC(2)$ 13.003354	$pC(2)$ 0.0111
H	$mH(1)$ 1.007825	$pH(1)$ 0.9999
	$mH(2)$ 2.014102	$pH(2)$ 0.0001
N	$mN(1)$ 14.003074	$pN(1)$ 0.9963
	$mN(2)$ 15.000108	$pN(2)$ 0.0037
O	$mO(1)$ 15.994915	$pO(1)$ 0.9976
	$mO(2)$ 16.999133	$pO(2)$ 0.0004
	$mO(3)$ 17.999160	$pO(3)$ 0.0020
S	$mS(1)$ 31.972074	$pS(1)$ 0.9502
	$mS(2)$ 32.971460	$pS(2)$ 0.0075
	$mS(3)$ 33.967864	$pS(3)$ 0.0422
	$mS(4)$ 35.967091	$pS(4)$ 0.0001

DETERMINATION OF FINAL ISOTOPE PEAK

OF THE ESTIMATED ISOTOPE PEAKS, AN INTENSITY DISTRIBUTION CALCULATED VALUE P_{Nis} OF ISOTOPE PEAKS AGREES WITH A RELATIVE VALUE OF A RELATIVE MEASURED INTENSITY FOR ISOTOPE-LESS PEAKS WITH AN ERROR OF LESS THAN 50%

FINALLY DETERMINE THE ESTIMATED ISOTOPE PEAK AS AN ISOTOPE PEAK

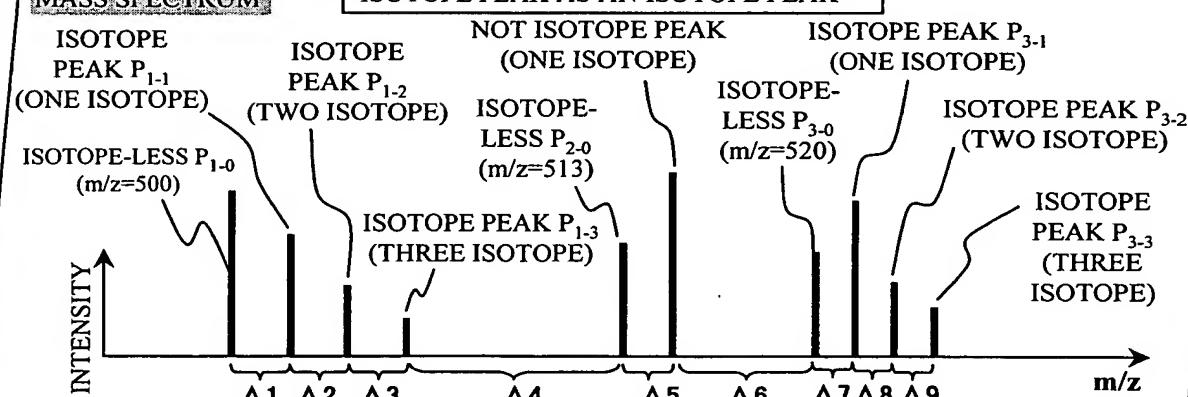


FIG. 10

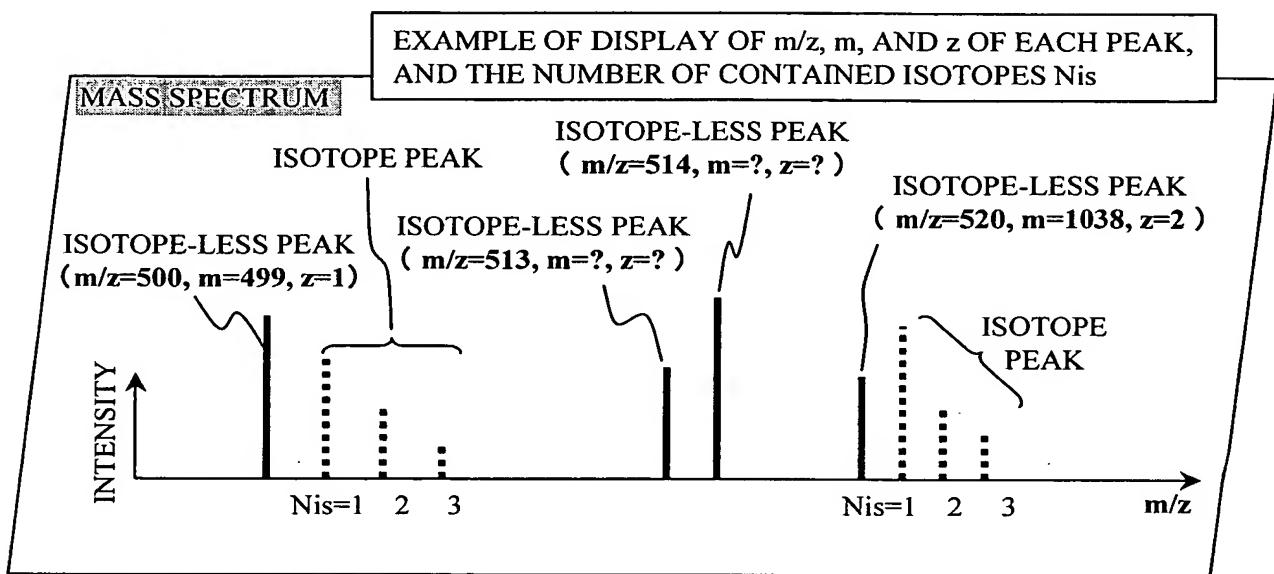


FIG. 11

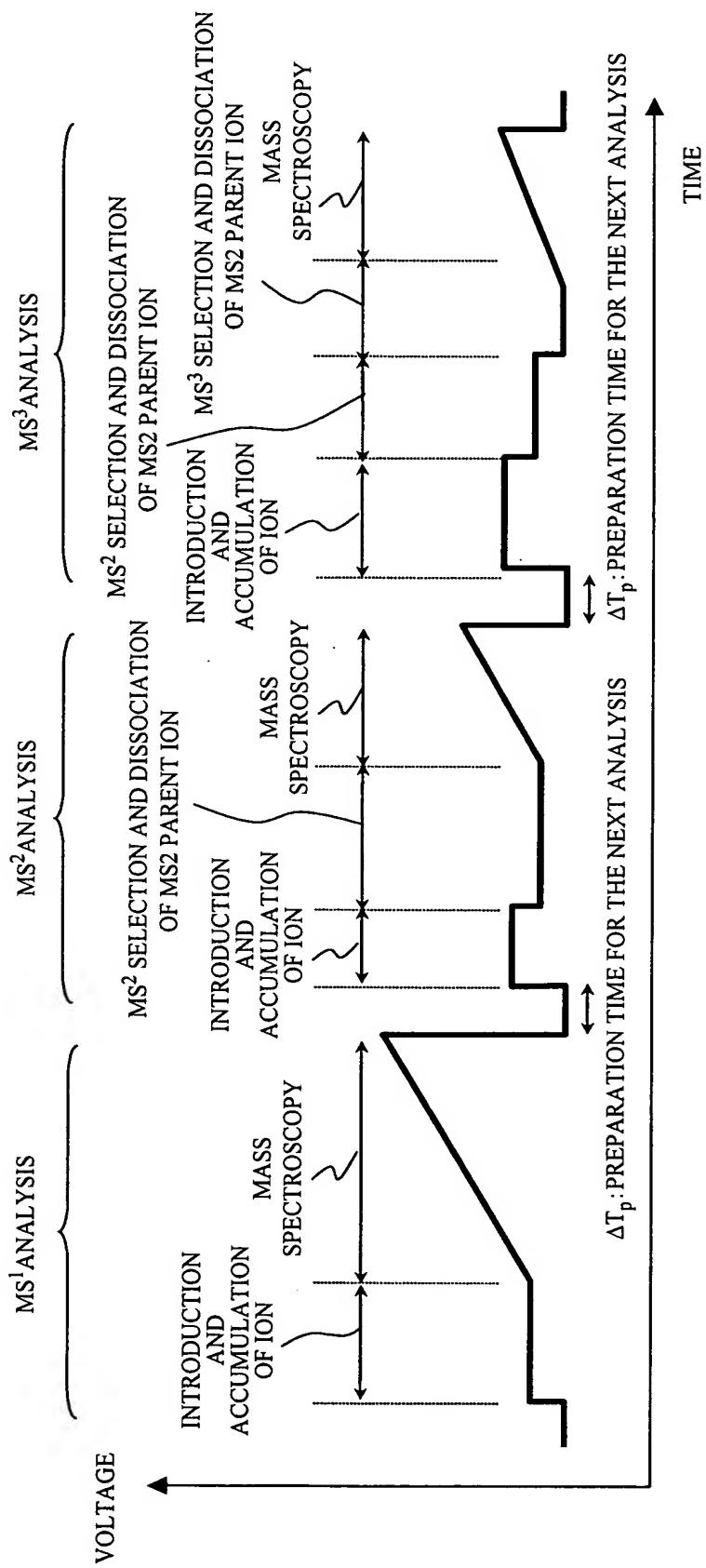


FIG. 12

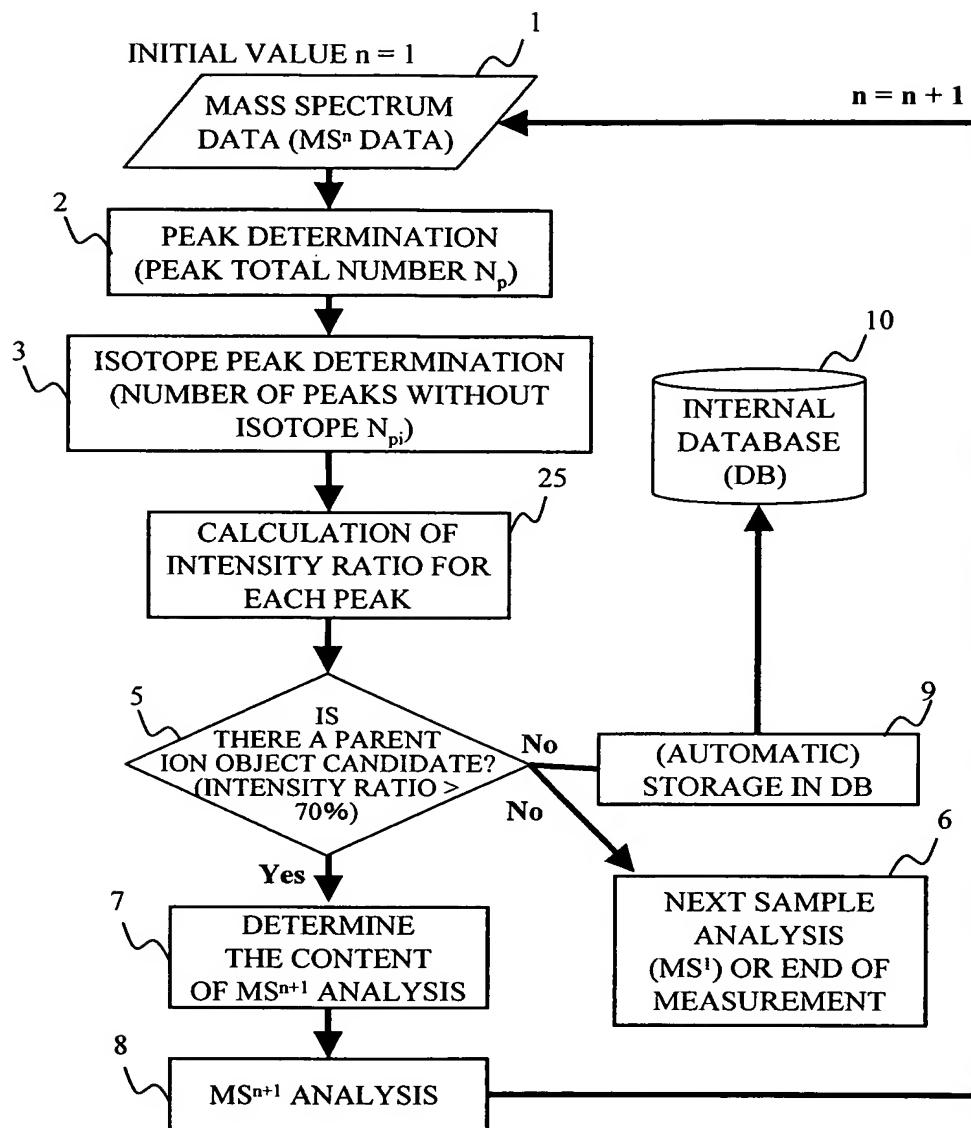


FIG. 13

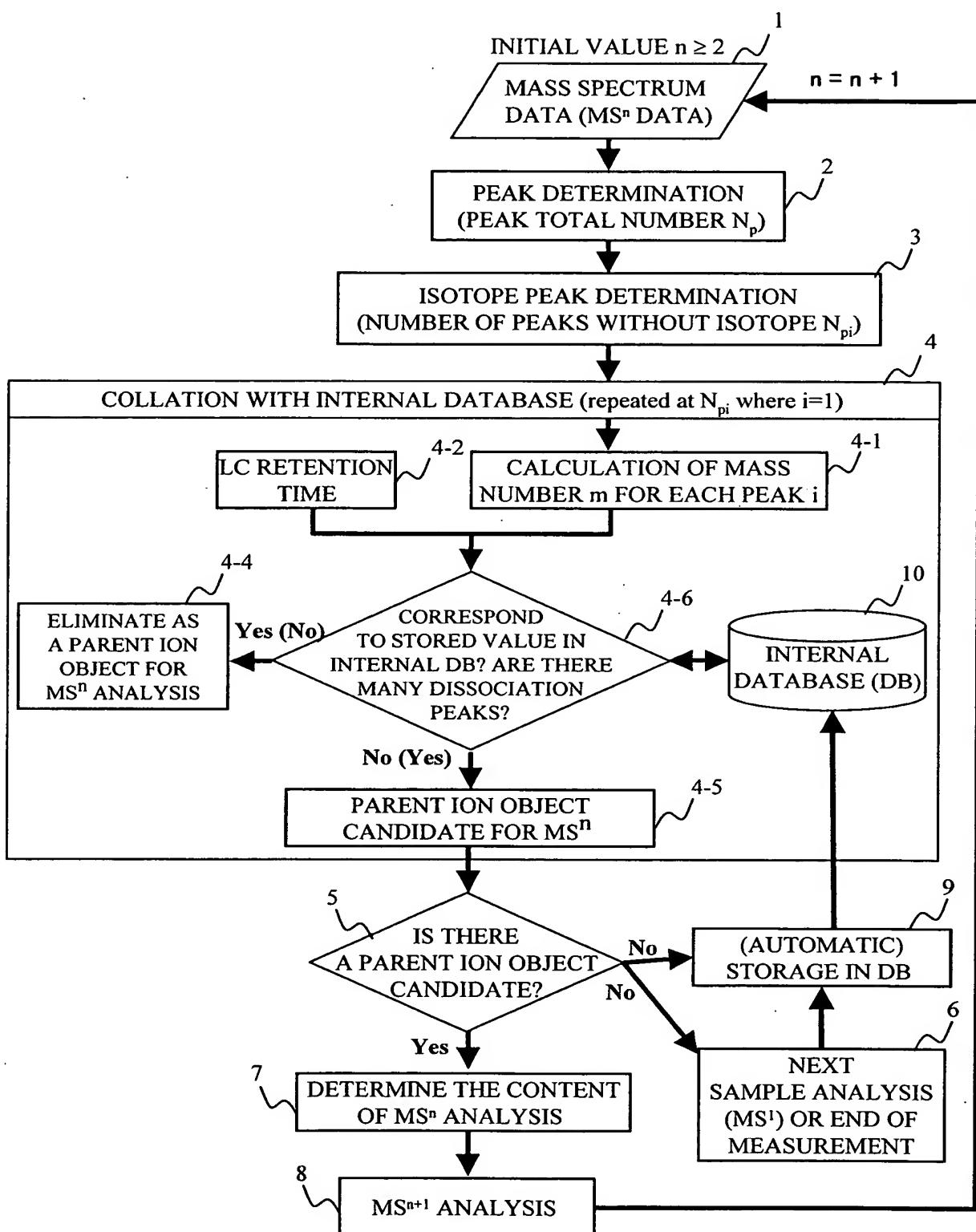


FIG. 14

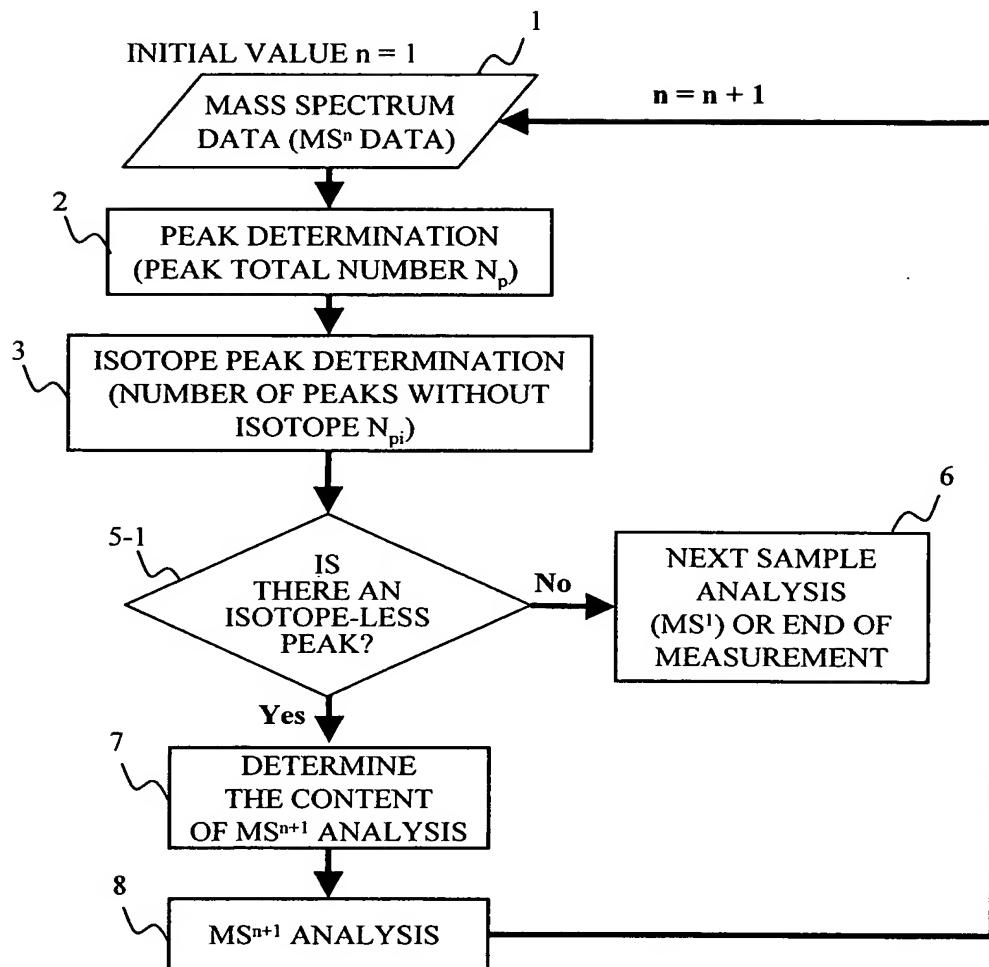


FIG. 15

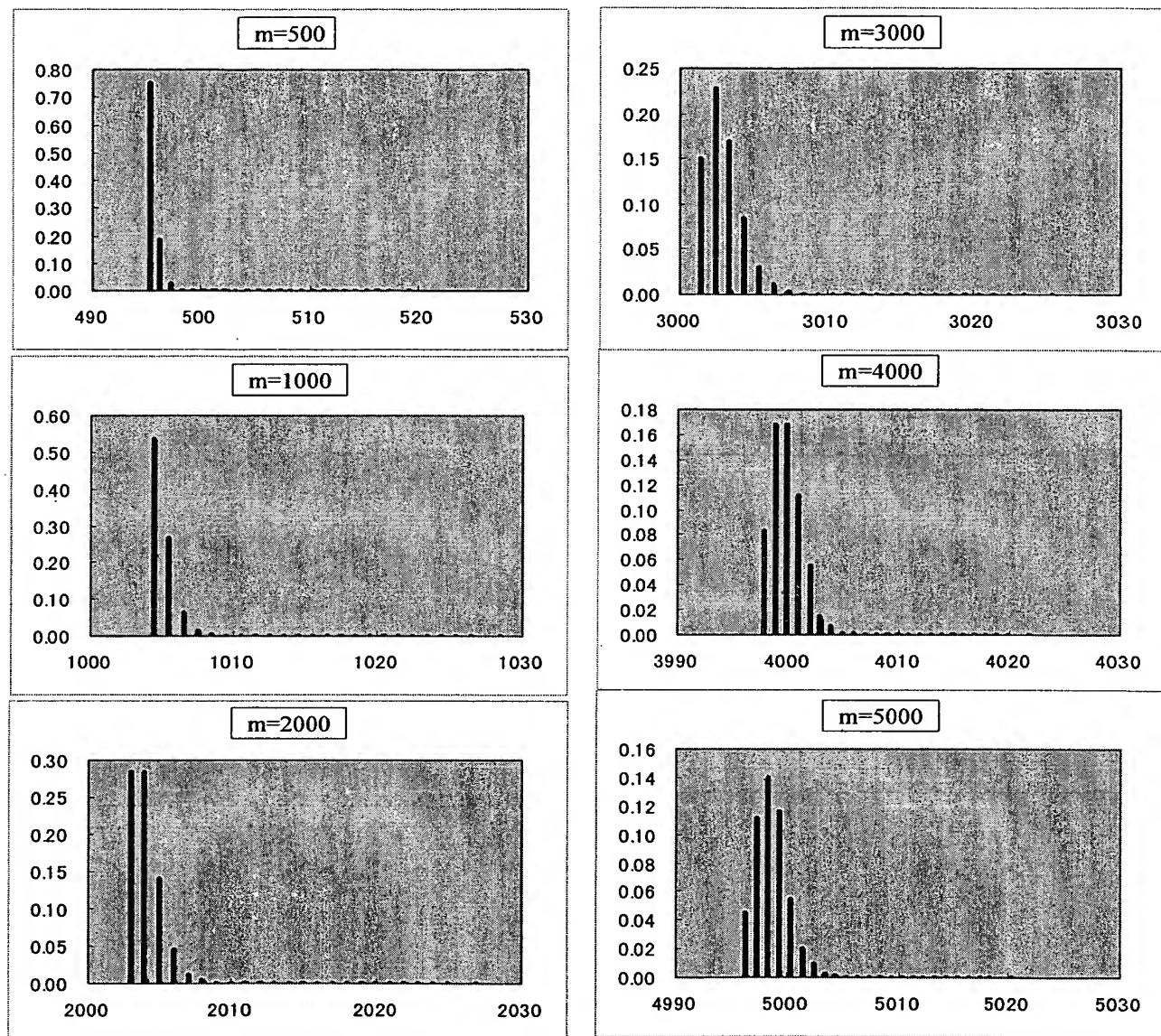
ISOTOPE PEAK INTENSITY DISTRIBUTION
PATTERNS DEPENDING ON ION MASS NUMBER

FIG. 16

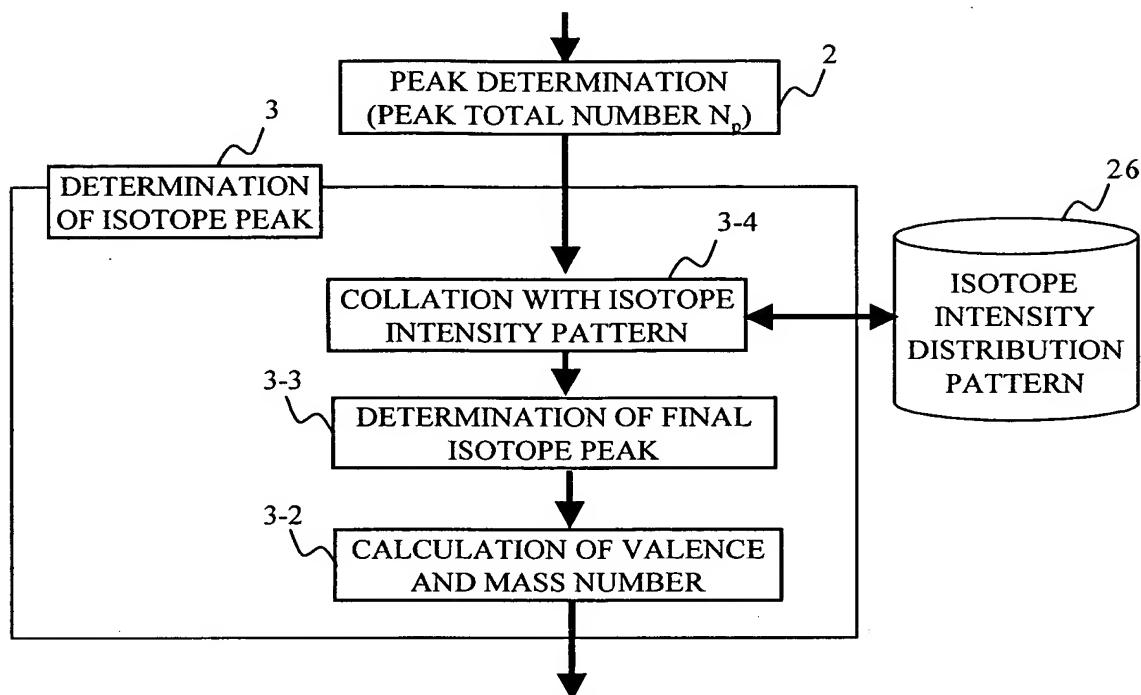


FIG. 17

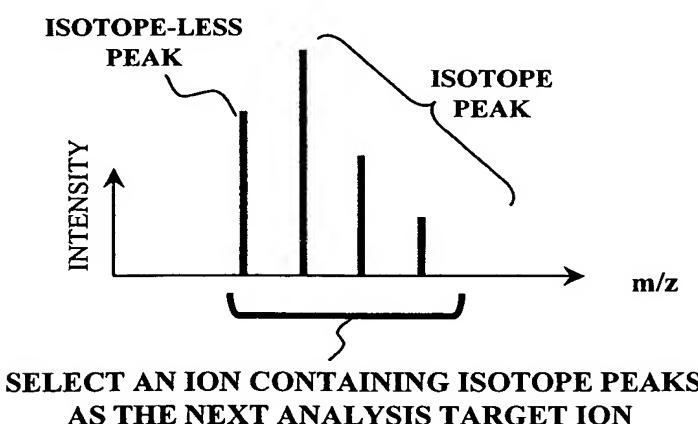


FIG. 18

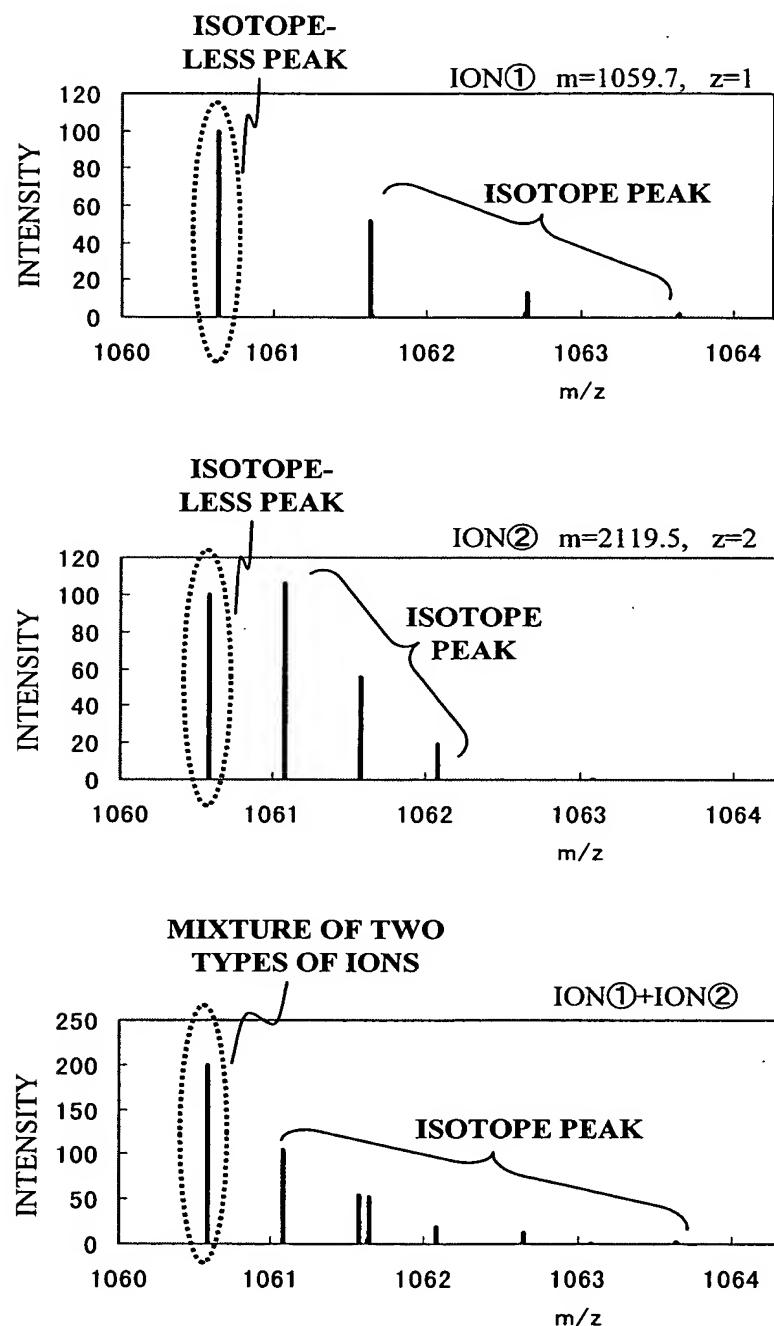


FIG. 19

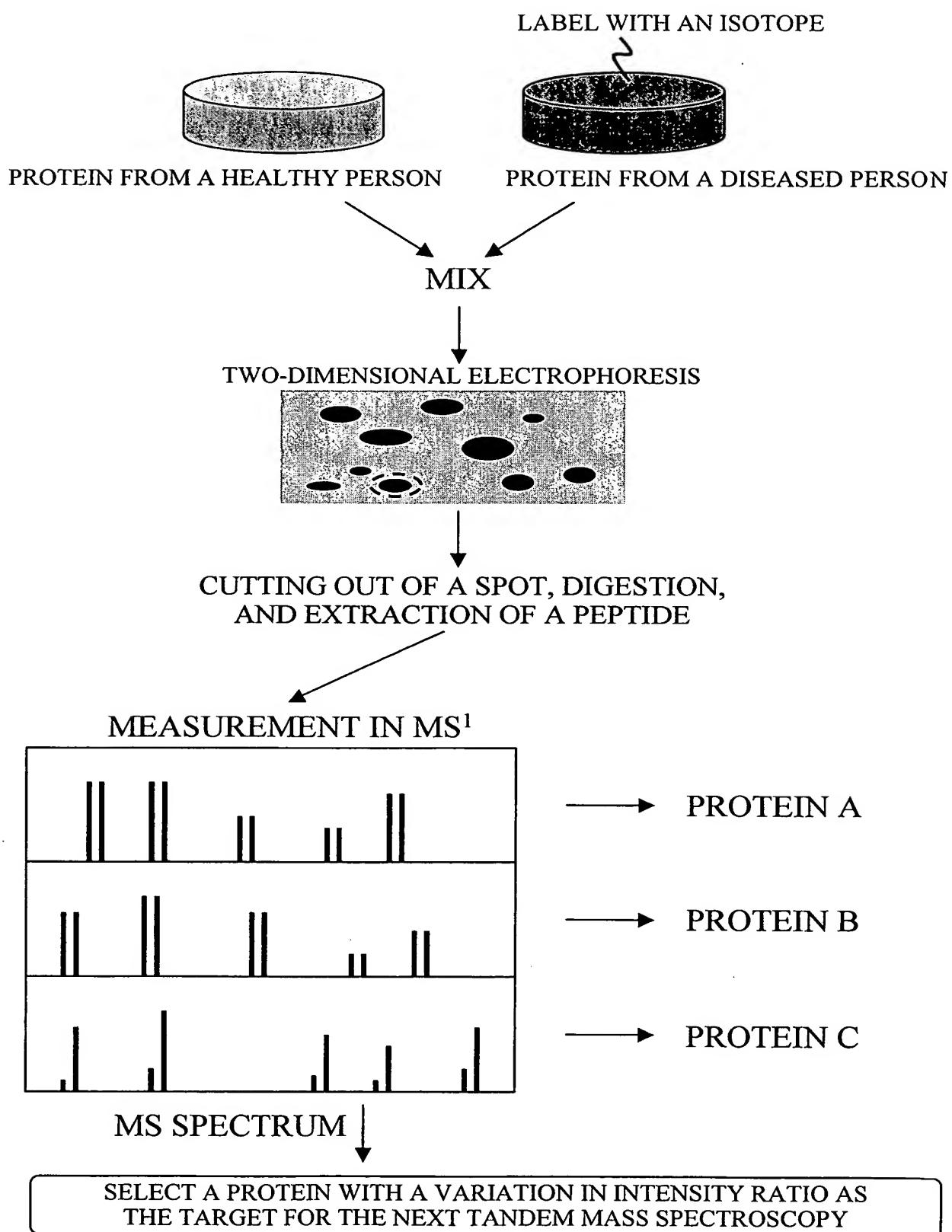


FIG. 20

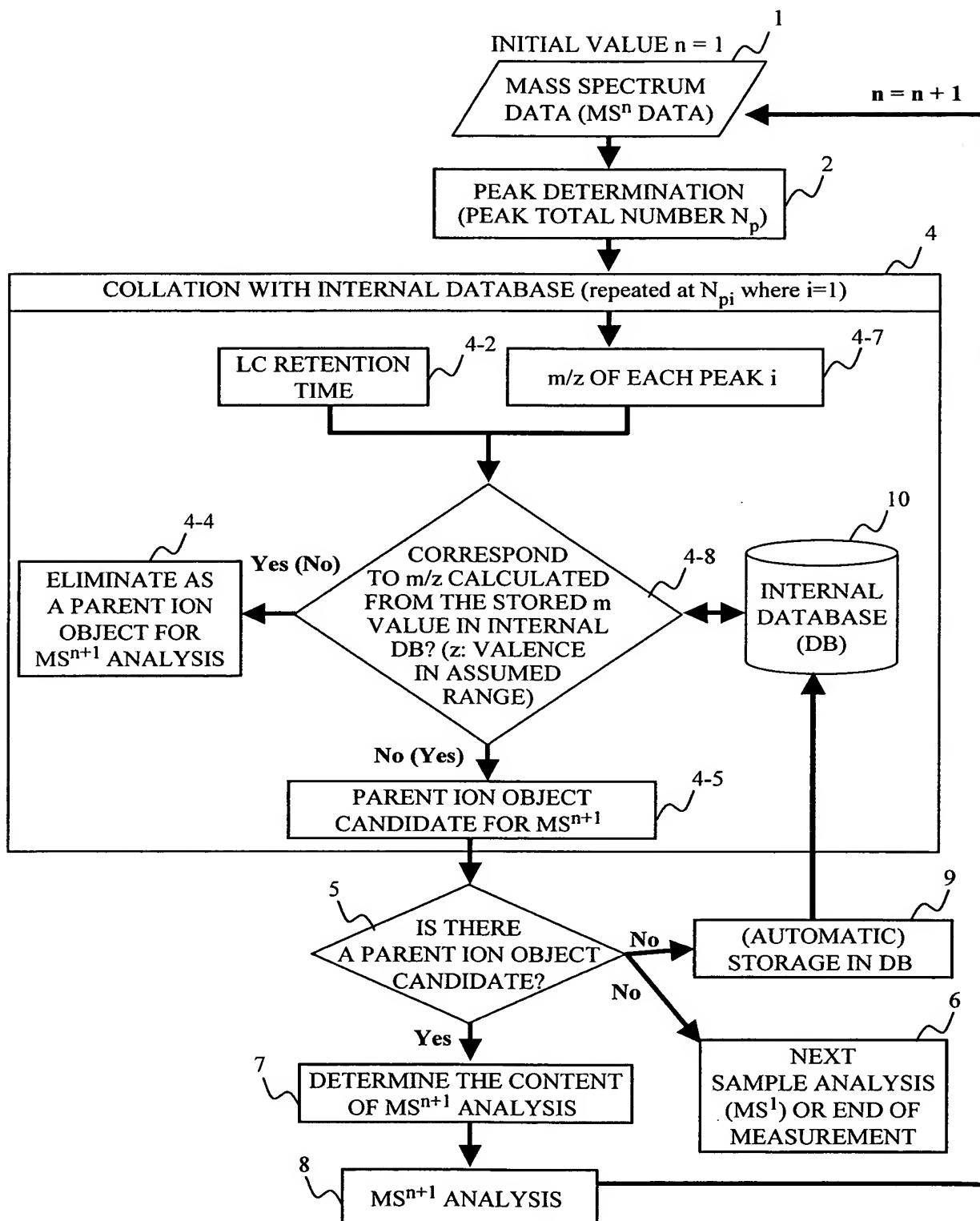


FIG. 21

MASS SPECTRUM

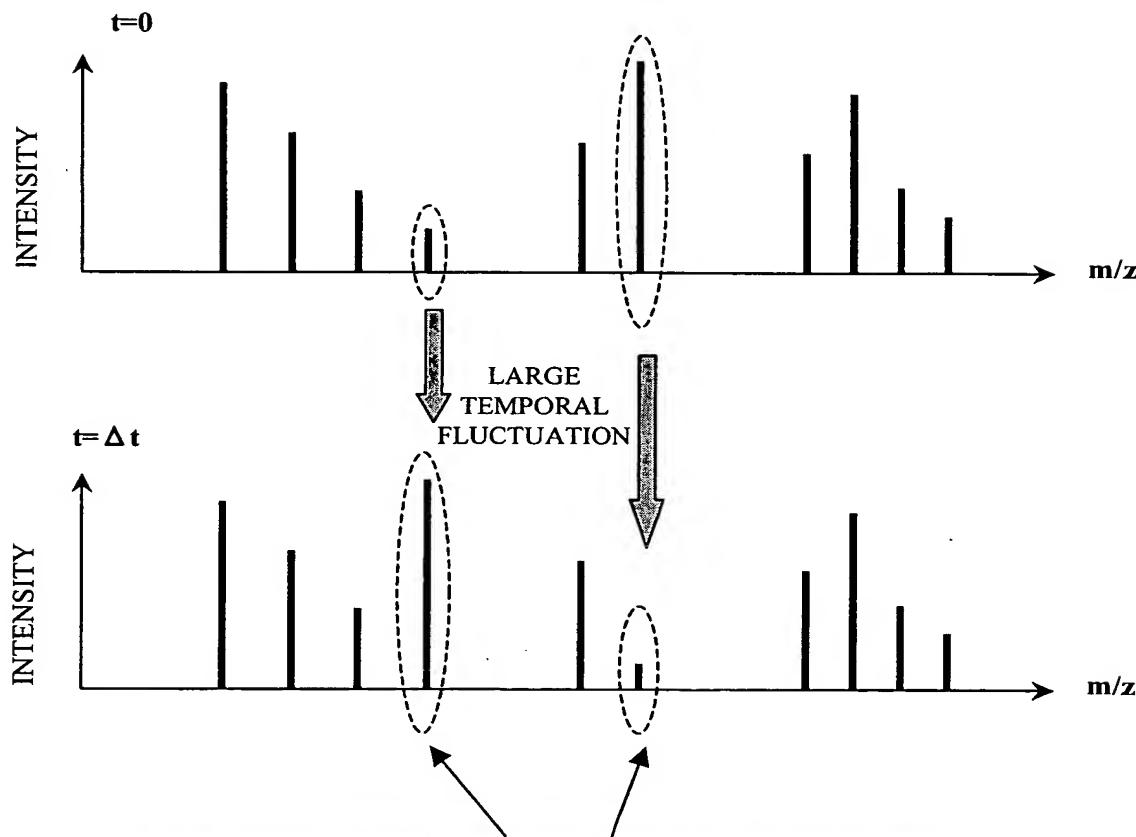


FIG. 22 a

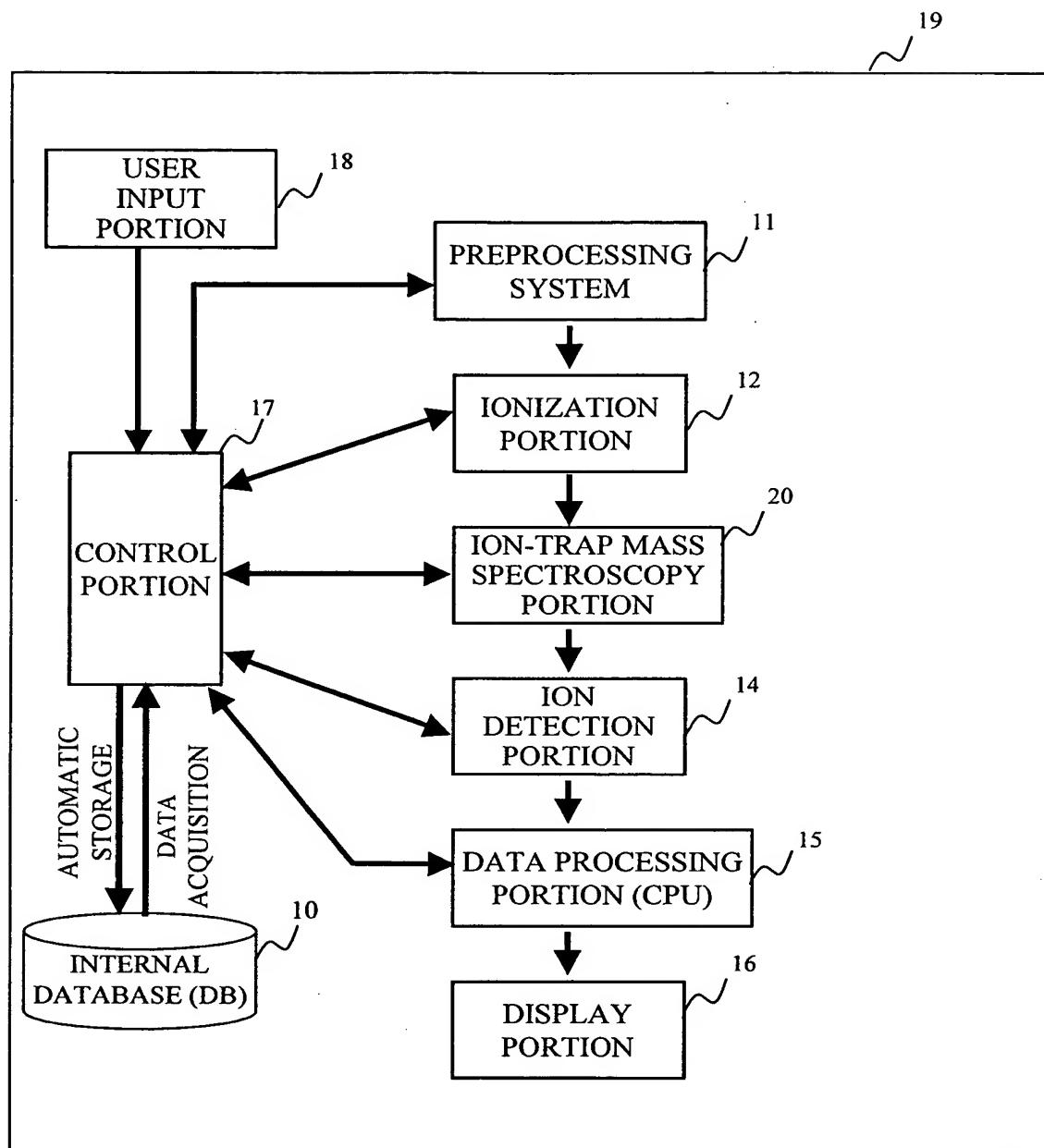


FIG. 22 b

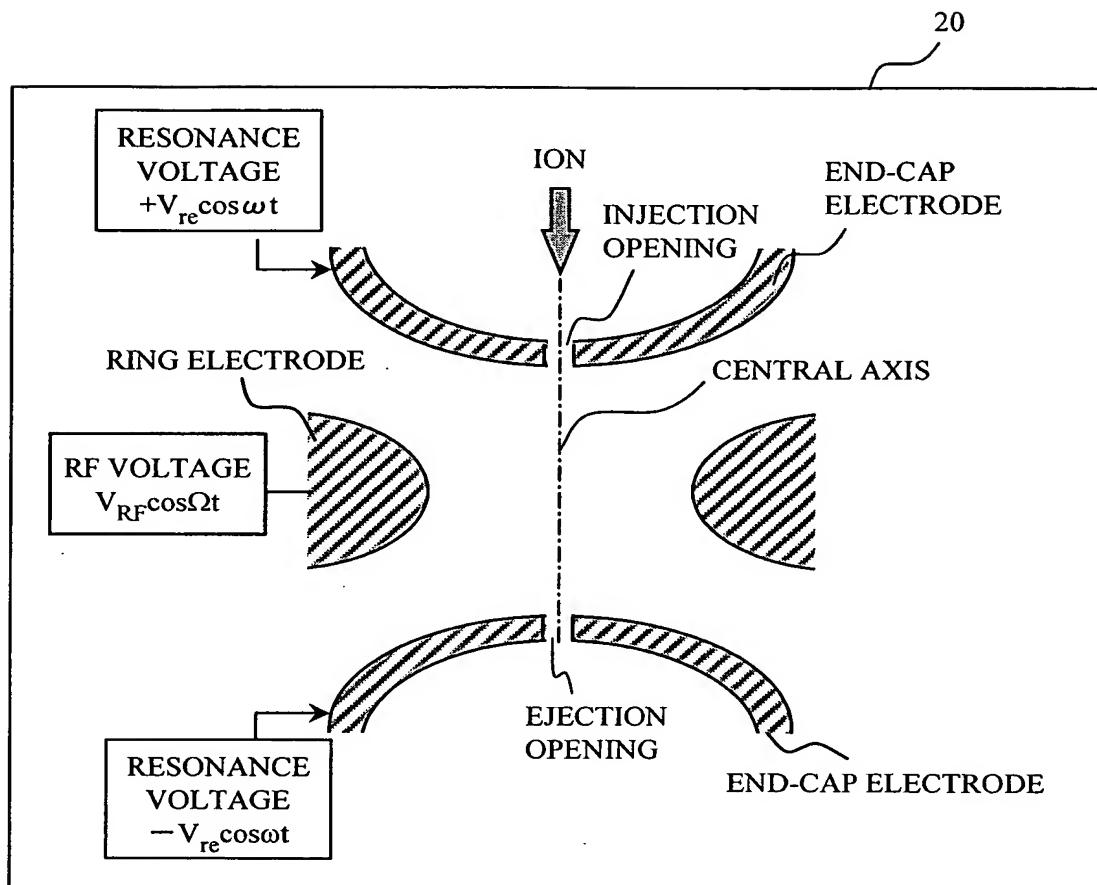


FIG. 23

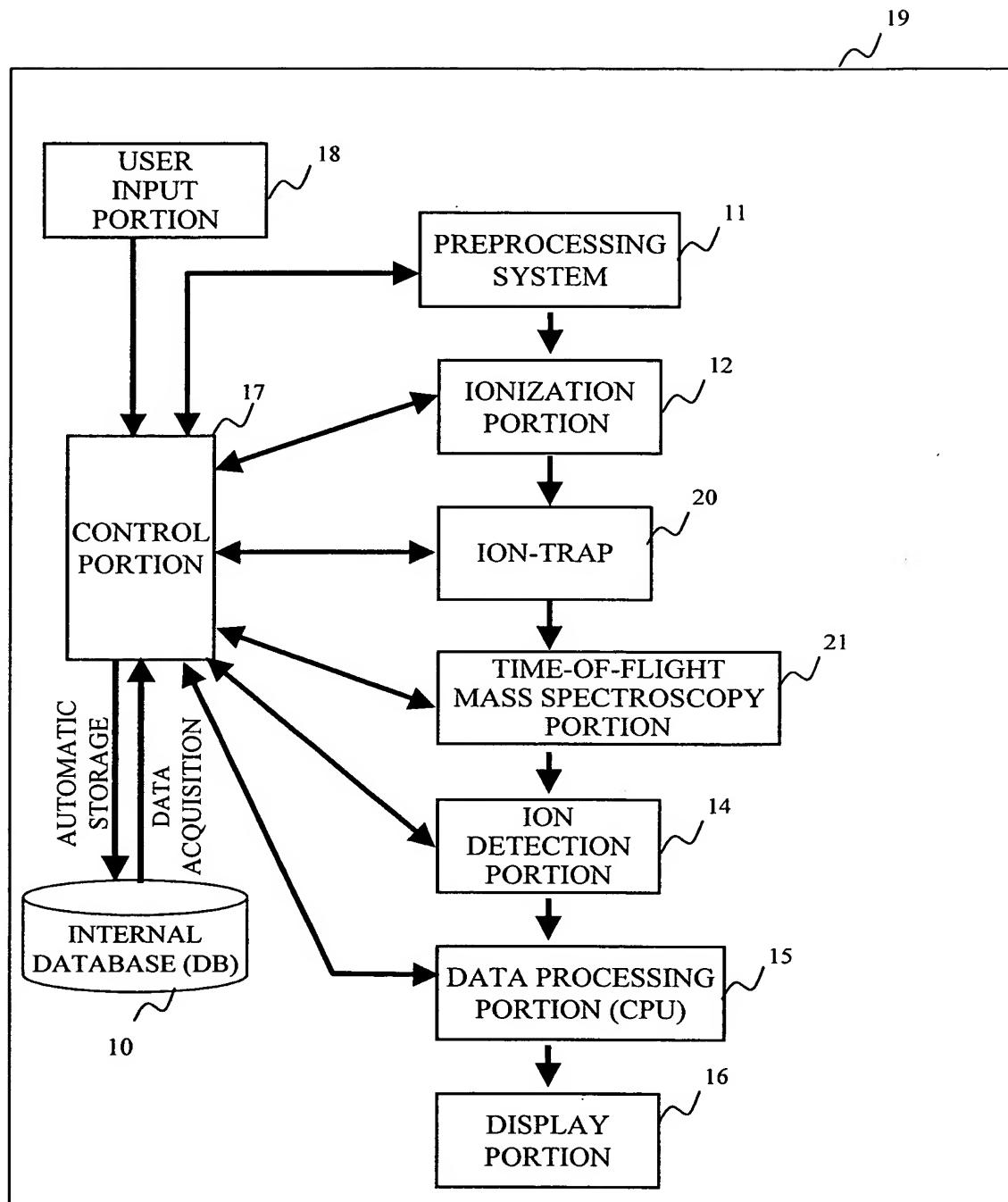


FIG. 24 a

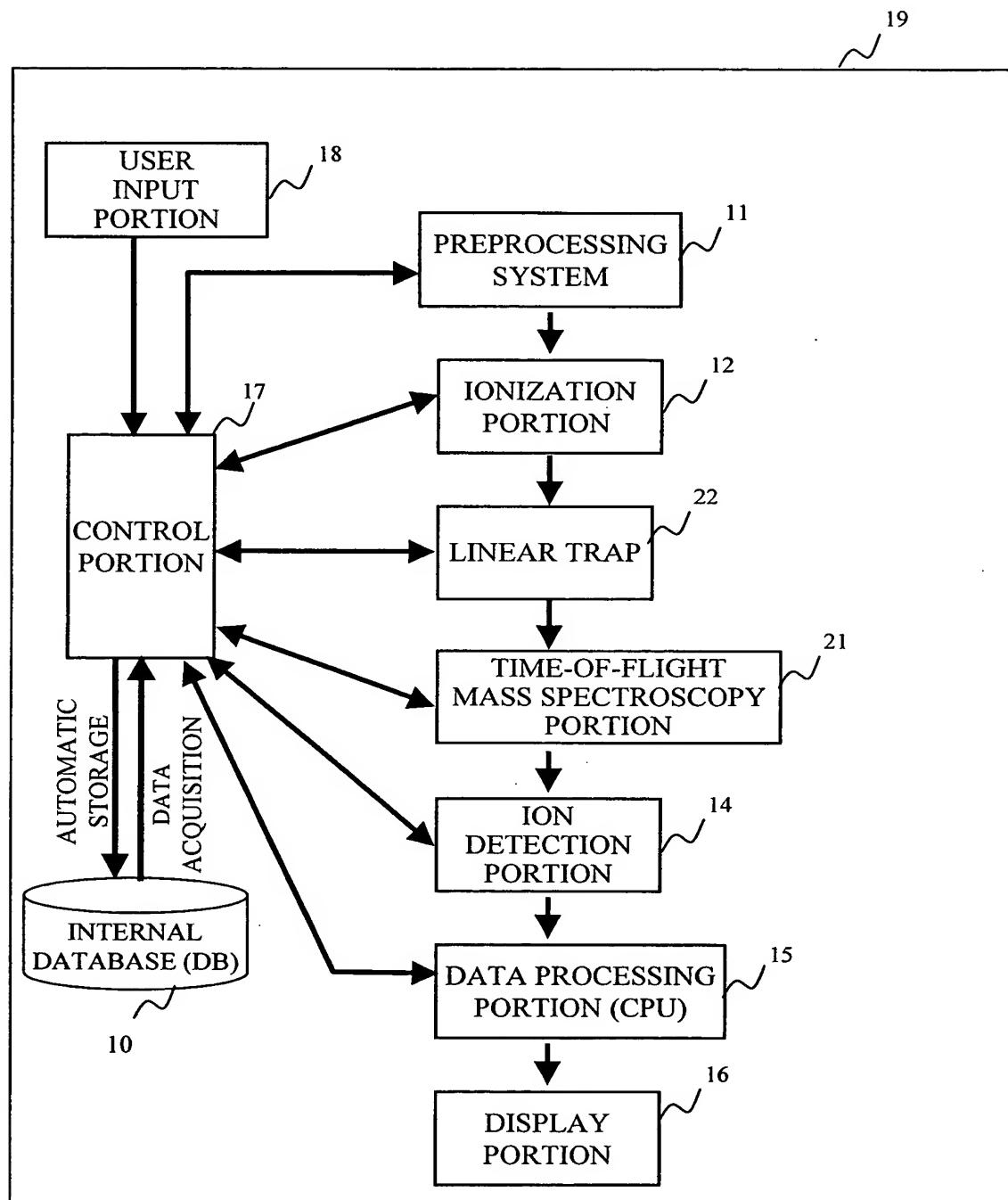


FIG. 24 b

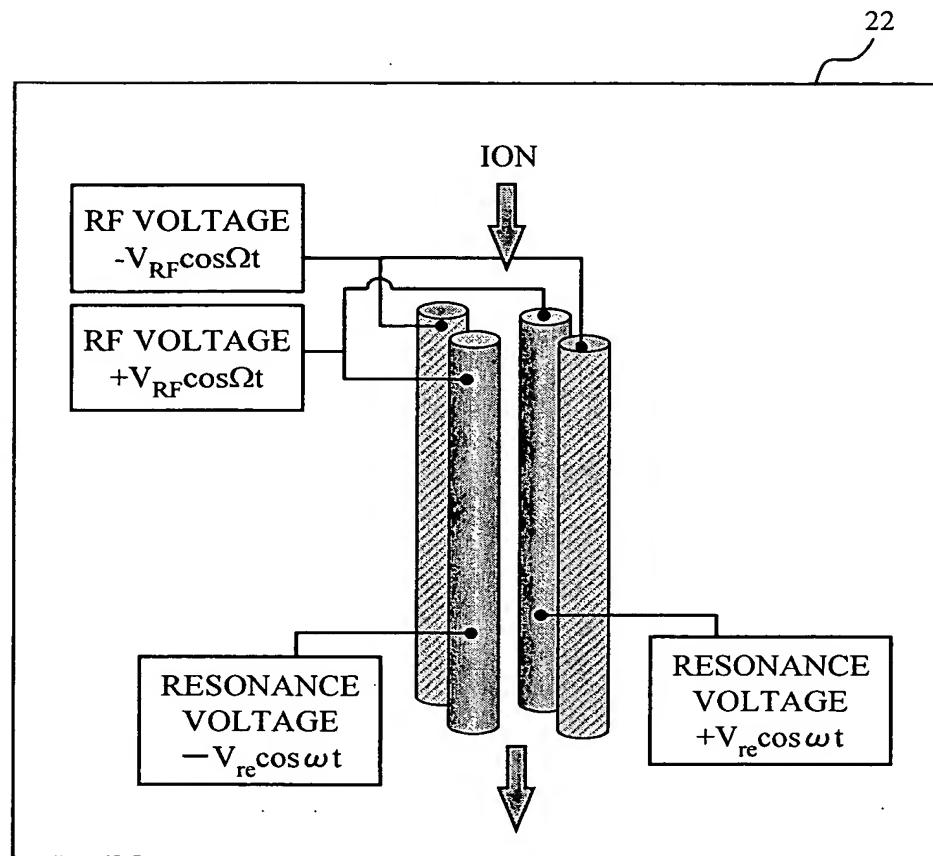


FIG. 25

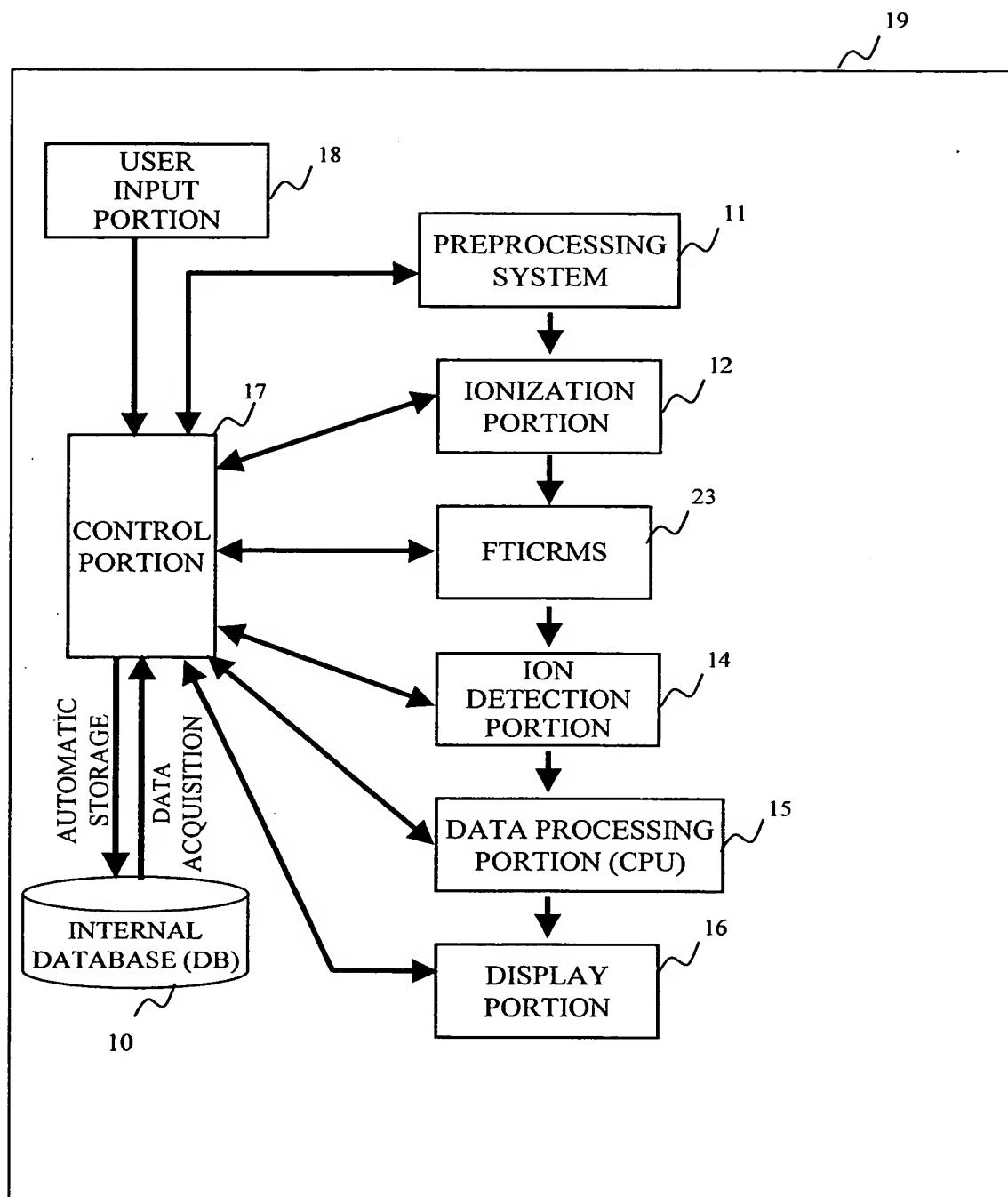


FIG. 26

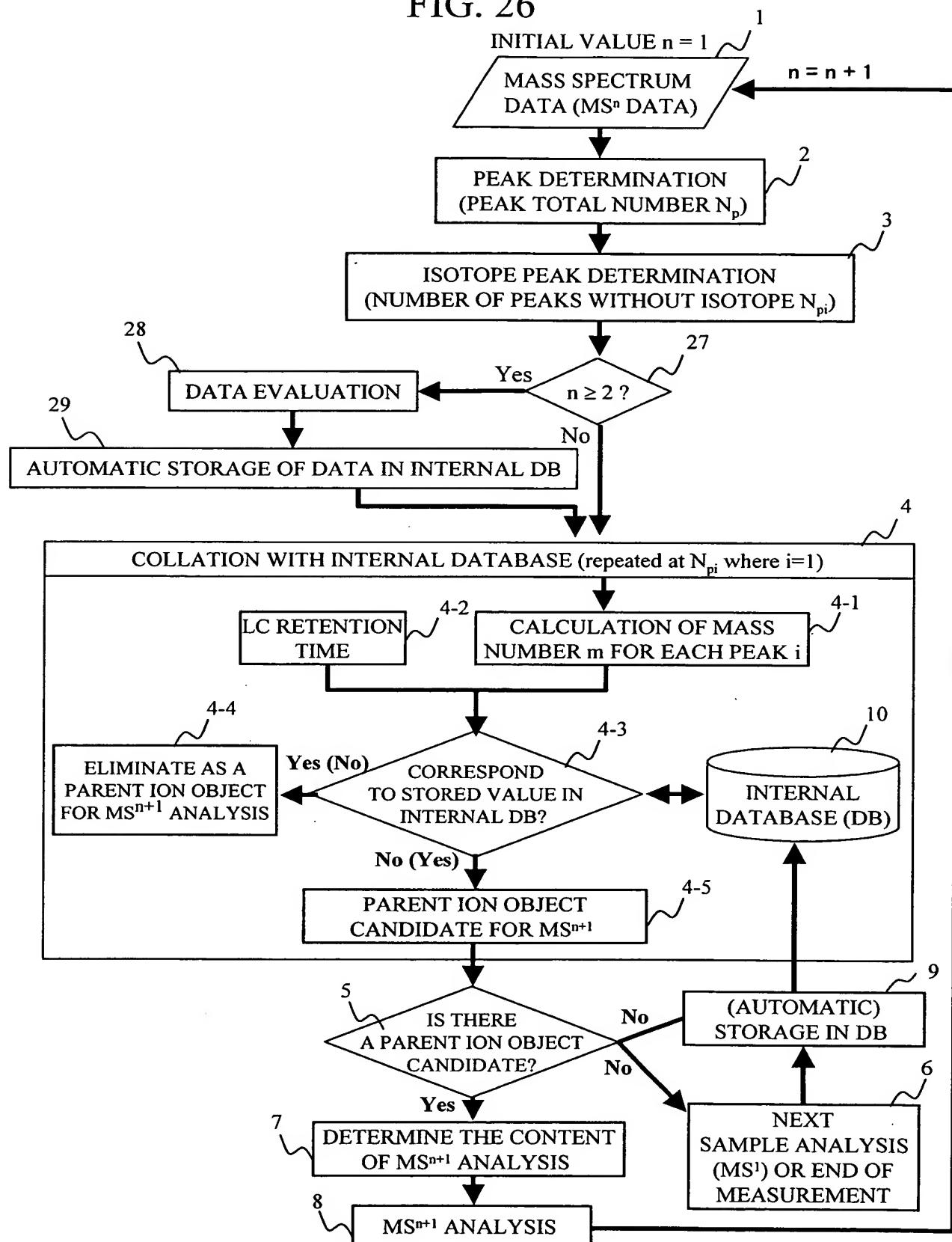


FIG. 27

INTERNAL DATABASE

No.	M [Da]	VALENCE z	τ [min]	Accumulation time[msec]	quality
1	921.23	2	24.5	260	5
2	926.09	2	26.9	345	4
3	973.26	2	32.0	289	4
4	700.39	2	34.1	401	5
5	480.66	2	39.2	269	3
6	582.29	2	44.7	159	2
7	1638.66	2	47.8	362	4
8	1954.86	3	50.8	410	5
9	507.8	2	51.1	359	5
10	CLICK 1510.54	2	57.6	190	3
11	740.25	2	59.8	278	5
12	1478.5	2	61.3	371	4
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

MASS SPECTRUM DATA DISPLAY

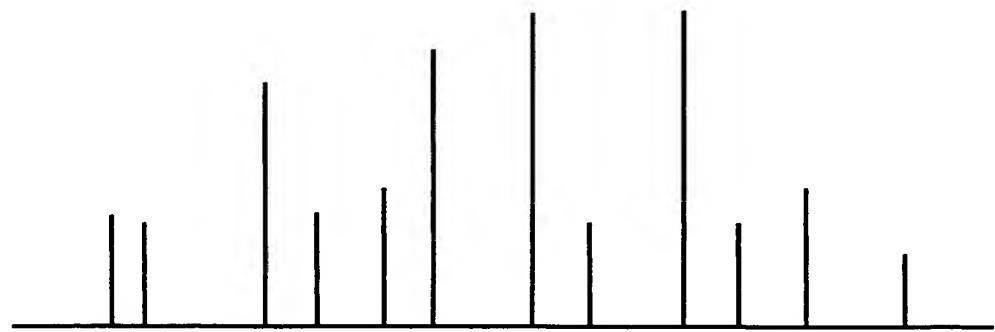


FIG. 28 A

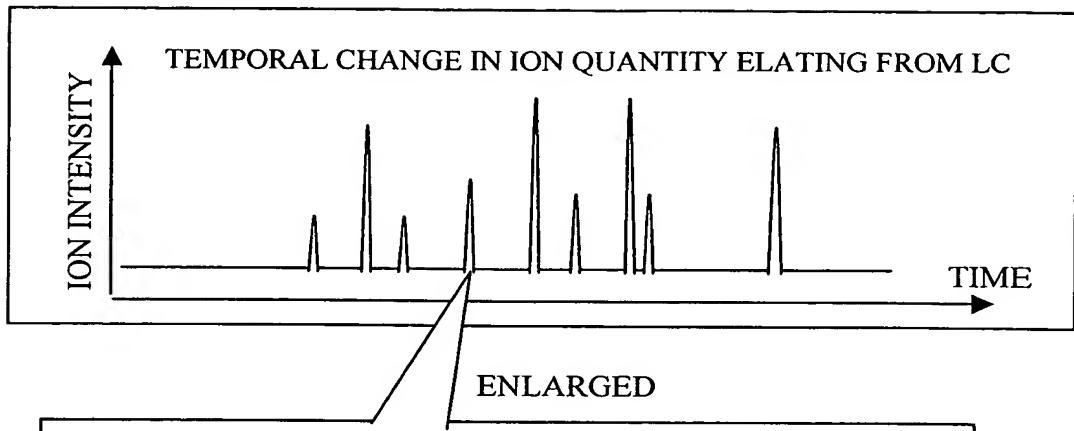


FIG. 28 B

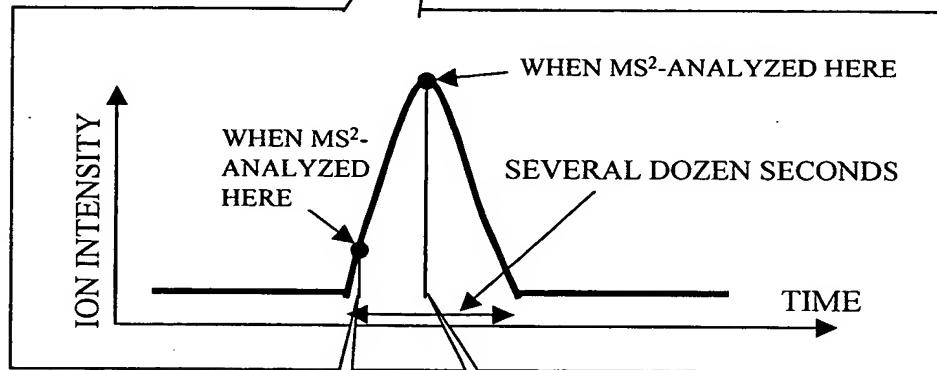


FIG. 28 C

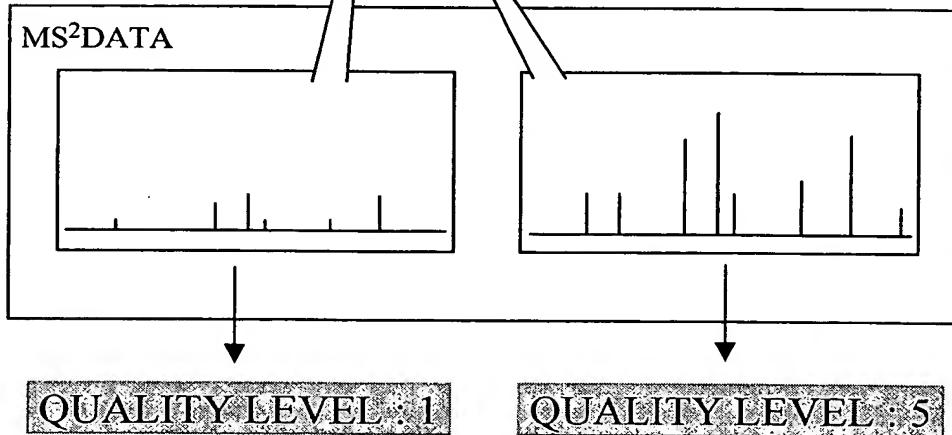


FIG. 29

INTERNAL DATABASE					
No.	M [Da]	VALENCE z	τ [min]	Accumulation time[msec]	quality
1	921.23	2	24.5	260	5
2	926.09	2	26.9	345	4
3	973.26	2	32.0	289	4
4	700.39	2	34.1	401	5
5	480.66	2	39.2	269	3
6	582.29	2	42.7	159	2
7	<u>1638.66</u>	<u>2</u>	<u>47.6</u>	362	2
8	<u>1638.67</u>	<u>2</u>	<u>47.7</u>	359	2
9	<u>1638.65</u>	<u>2</u>	<u>47.7</u>	339	3
10	<u>1638.66</u>	<u>2</u>	<u>47.7</u>	352	3
11	<u>1638.67</u>	<u>2</u>	<u>47.8</u>	254	4
12	<u>1638.68</u>	<u>2</u>	<u>47.8</u>	262	5
13	<u>1638.66</u>	<u>2</u>	<u>47.8</u>	219	5
14	<u>1638.65</u>	<u>2</u>	<u>47.8</u>	285	4
15	<u>1638.66</u>	<u>2</u>	<u>47.8</u>	248	5
16	<u>1638.65</u>	<u>2</u>	<u>47.8</u>	299	4
17	<u>1638.68</u>	<u>2</u>	<u>47.9</u>	280	4
18	<u>1638.67</u>	<u>2</u>	<u>47.9</u>	310	3
19	<u>1638.67</u>	<u>2</u>	<u>48.0</u>	307	3
20	<u>1638.64</u>	<u>2</u>	<u>48.0</u>	336	3
21	<u>1638.65</u>	<u>2</u>	<u>48.0</u>	318	3
22	1954.86	3	50.8	410	5
23	507.8	2	51.1	359	5
24	1510.54	2	57.6	190	3
25	740.25	2	59.8	278	5
26	1478.5	2	61.3	371	4
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

CAN BE CONSIDERED
AS IDENTICAL ION
(BASED ON MASS
NUMBER, VALENCE,
AND RETENTION TIME)

DELETE REDUNDANT
DATA FROM DB

FIG. 30

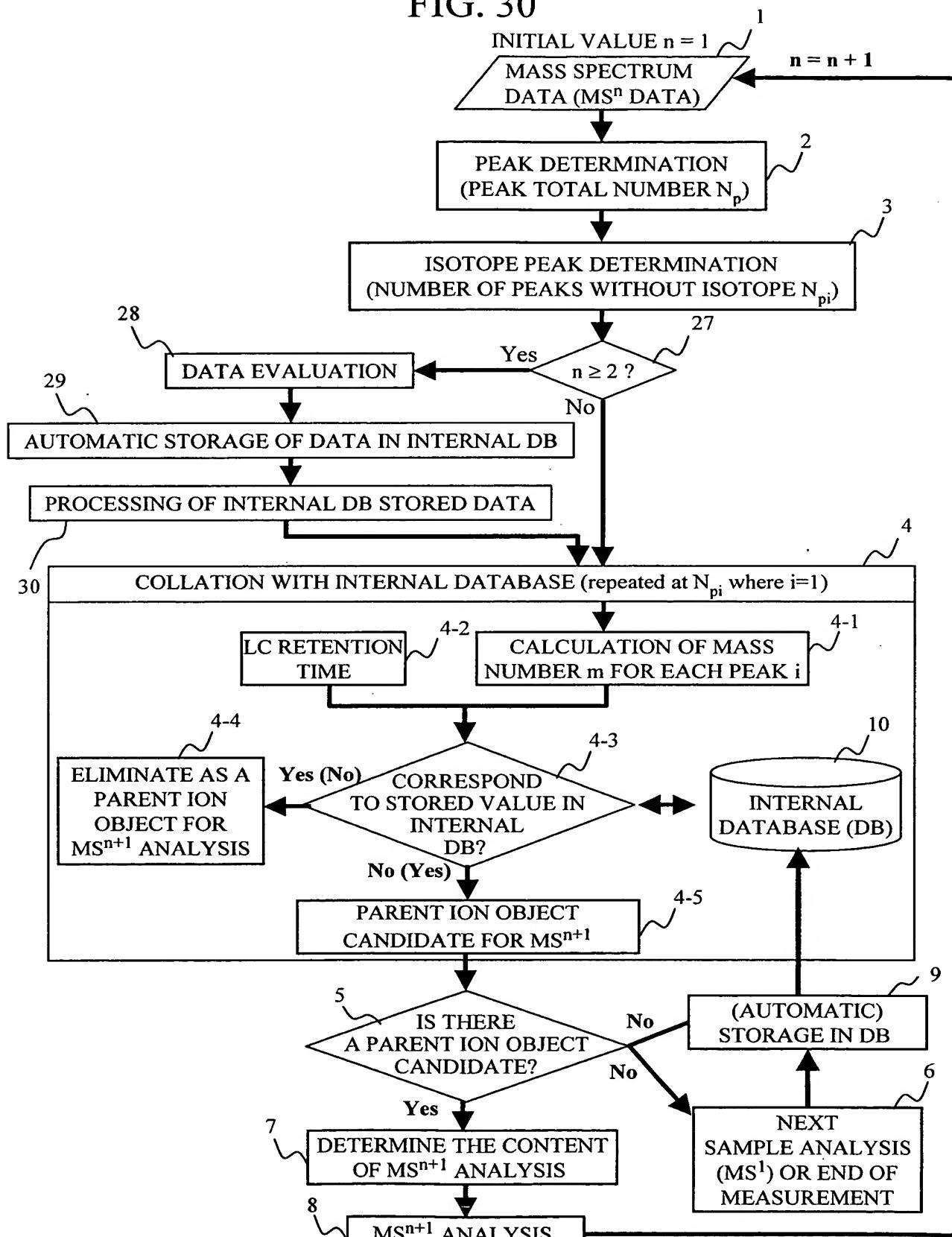


FIG. 31

INTERNAL DATABASE

No.	M [Da]	VALENCE z	τ [min]	Accumulation time [msec]	quality
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
N	1638.67	2	47.7	359	3
N+1	838.68	1	47.7	439	2
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

MS² ANALYSIS

MS³ ANALYSIS

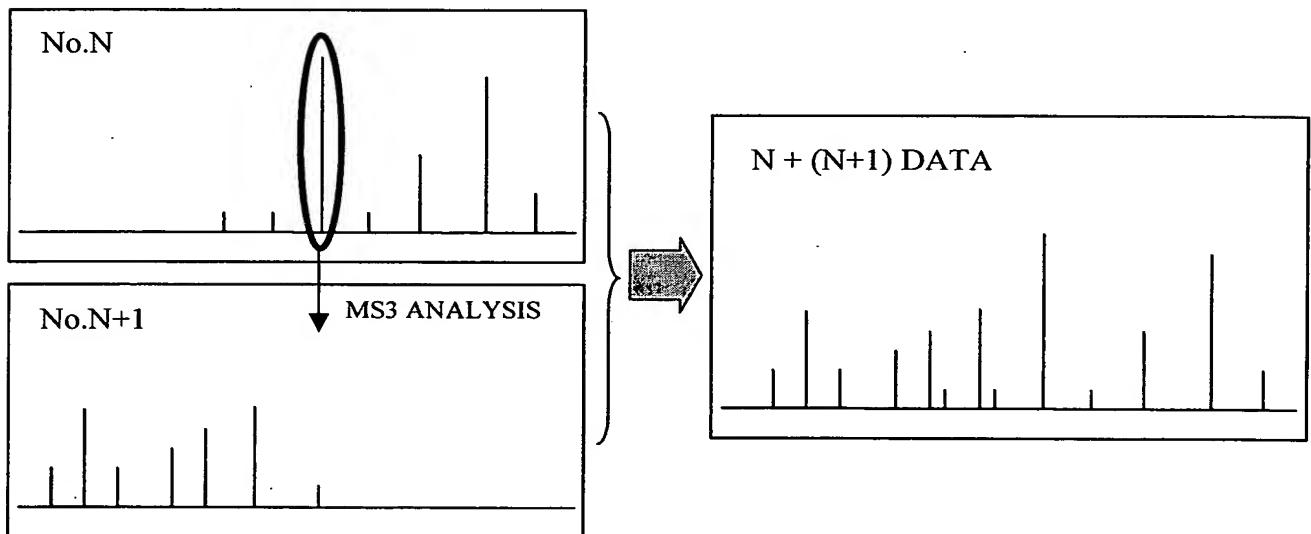


FIG. 32

INTERNAL DATABASE

No.	M [Da]	VALENCE z	τ [min]	Accumulation time [msec]	quality
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
K	1638.67	2	47.7	359	3
K+1	1638.68	2	47.7	339	3
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•
•	•	•	•	•	•

DATA DUE TO COLLISION INDUCED DISSOCIATION (CID)

DATA DUE TO ELECTRON CAPTURE DISSOCIATION (ECD)

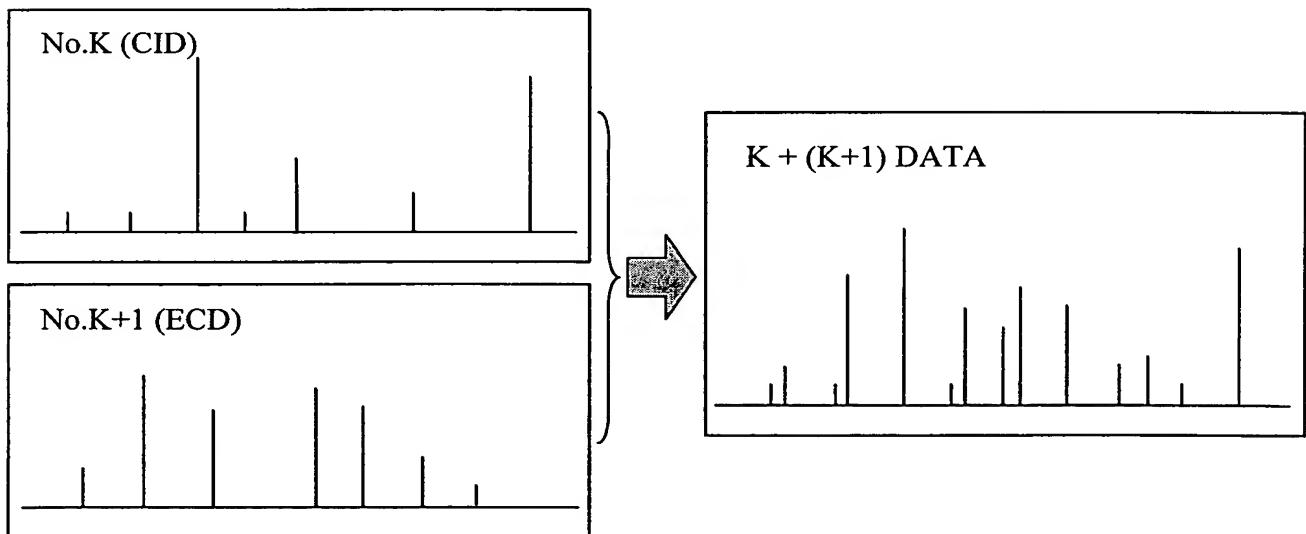


FIG. 33

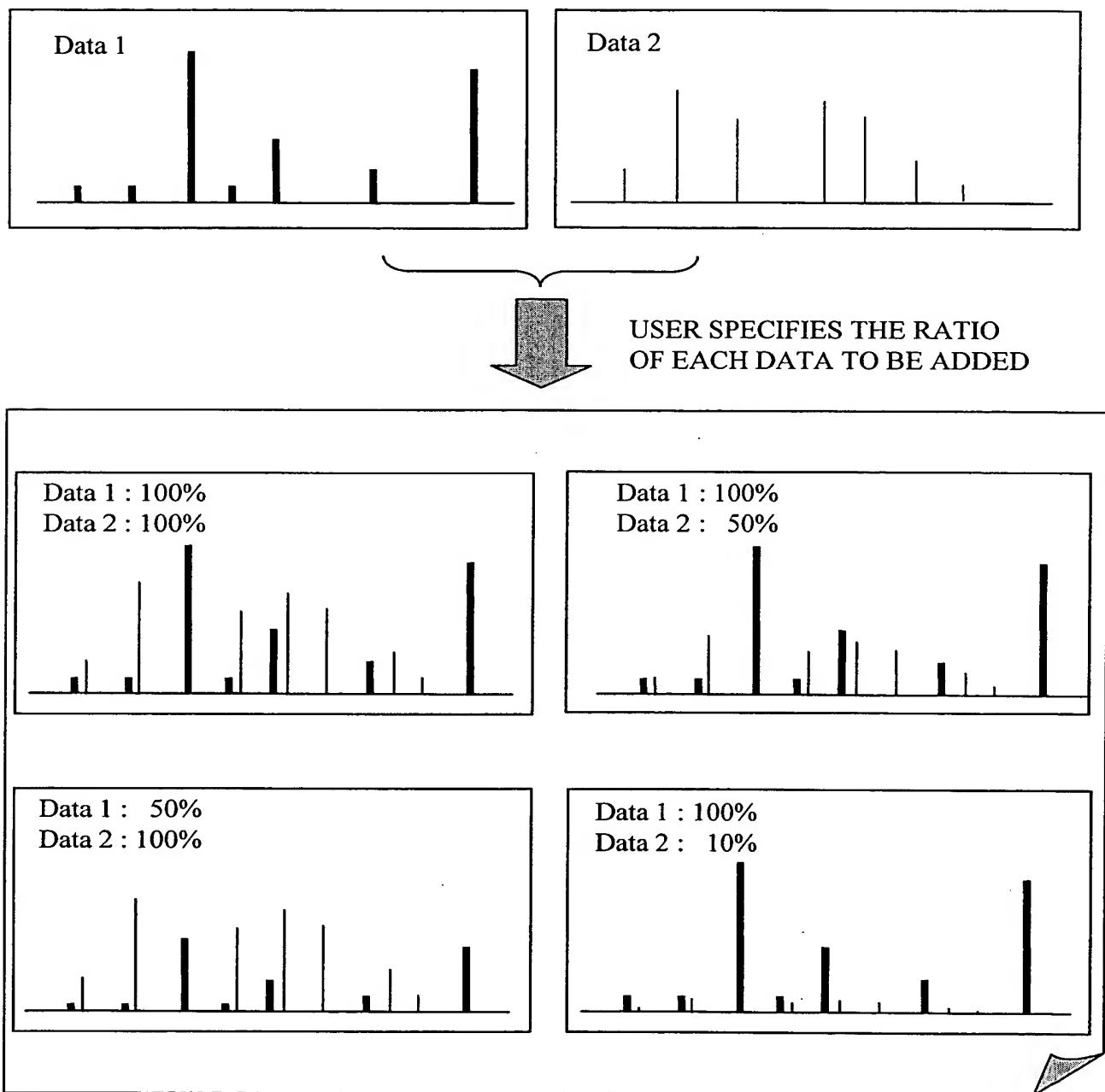
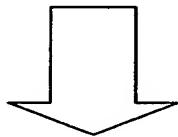
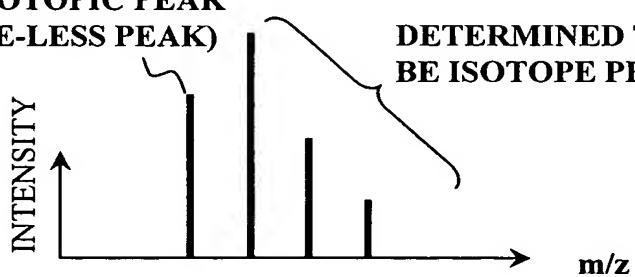


FIG. 34

**MONOISOTOPIC PEAK
(ISOTOPE-LESS PEAK)**



**MONOISOTOPIC PEAK
(ISOTOPE-LESS PEAK)**

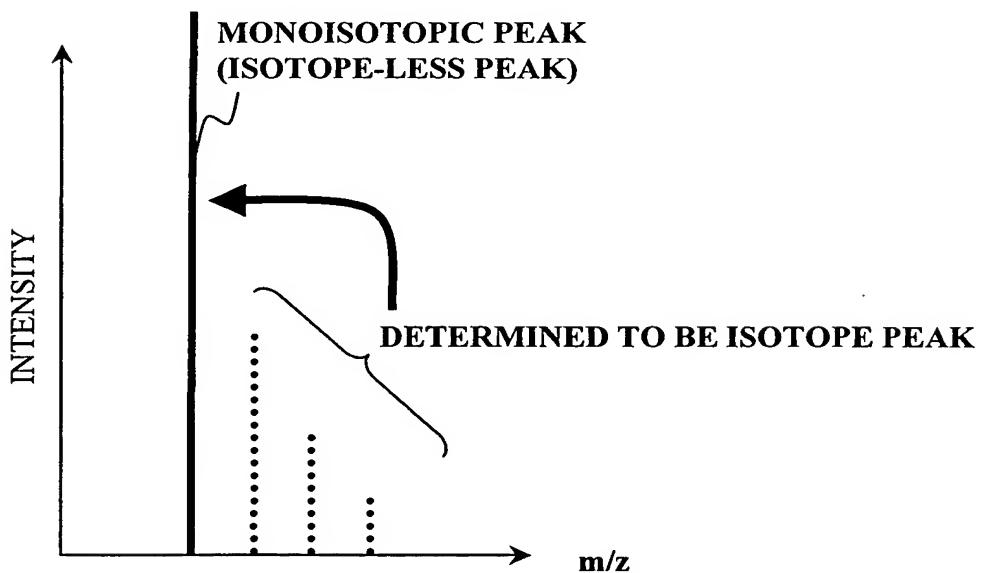


FIG. 35 a

PROTEIN ANALYSIS AND IDENTIFICATION FLOW IN PRIOR ART

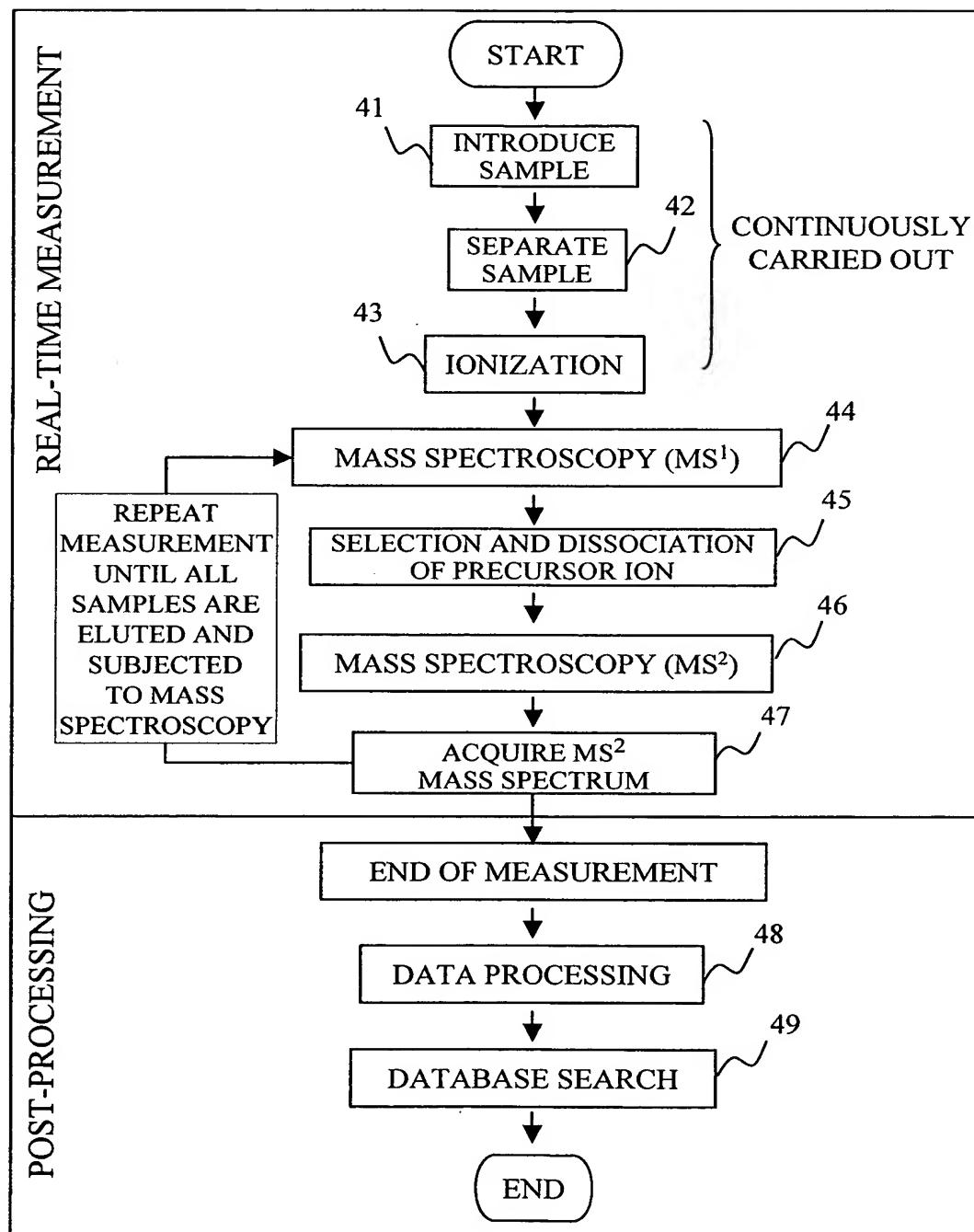


FIG. 35 b

PROTEIN ANALYSIS AND IDENTIFICATION FLOW IN THE PRESENT EMBODIMENT

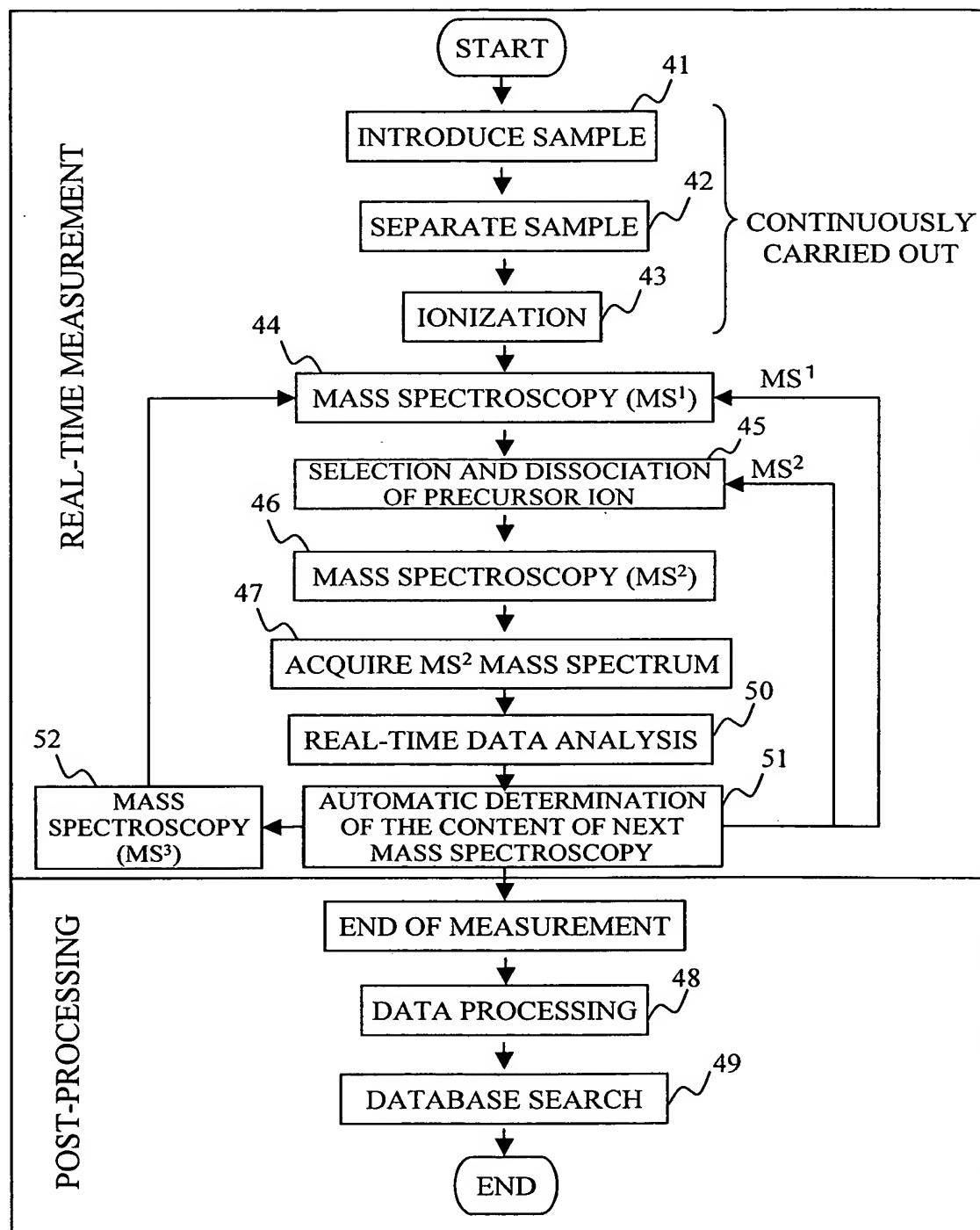


FIG. 36

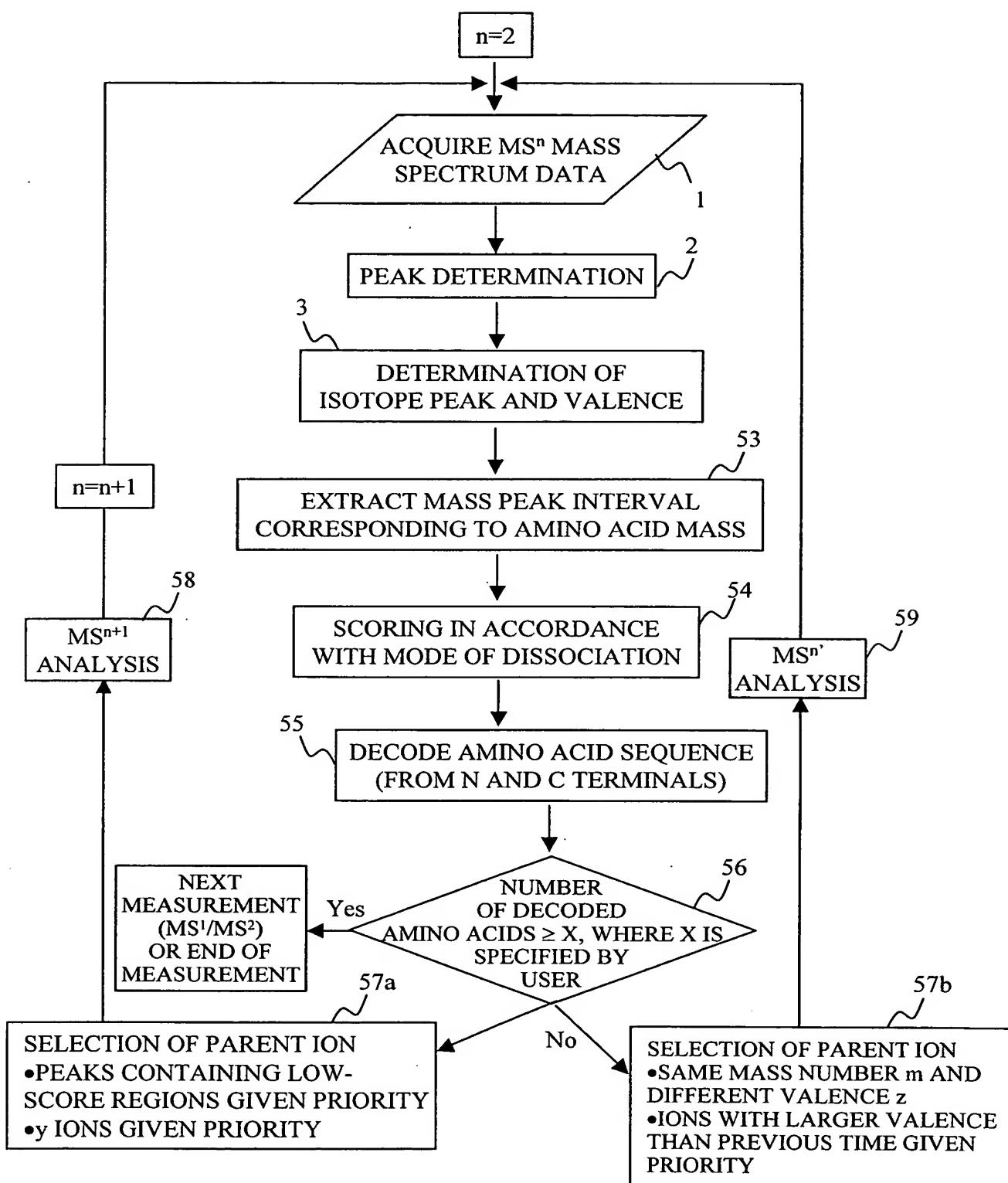


FIG. 37

MIFVGIK

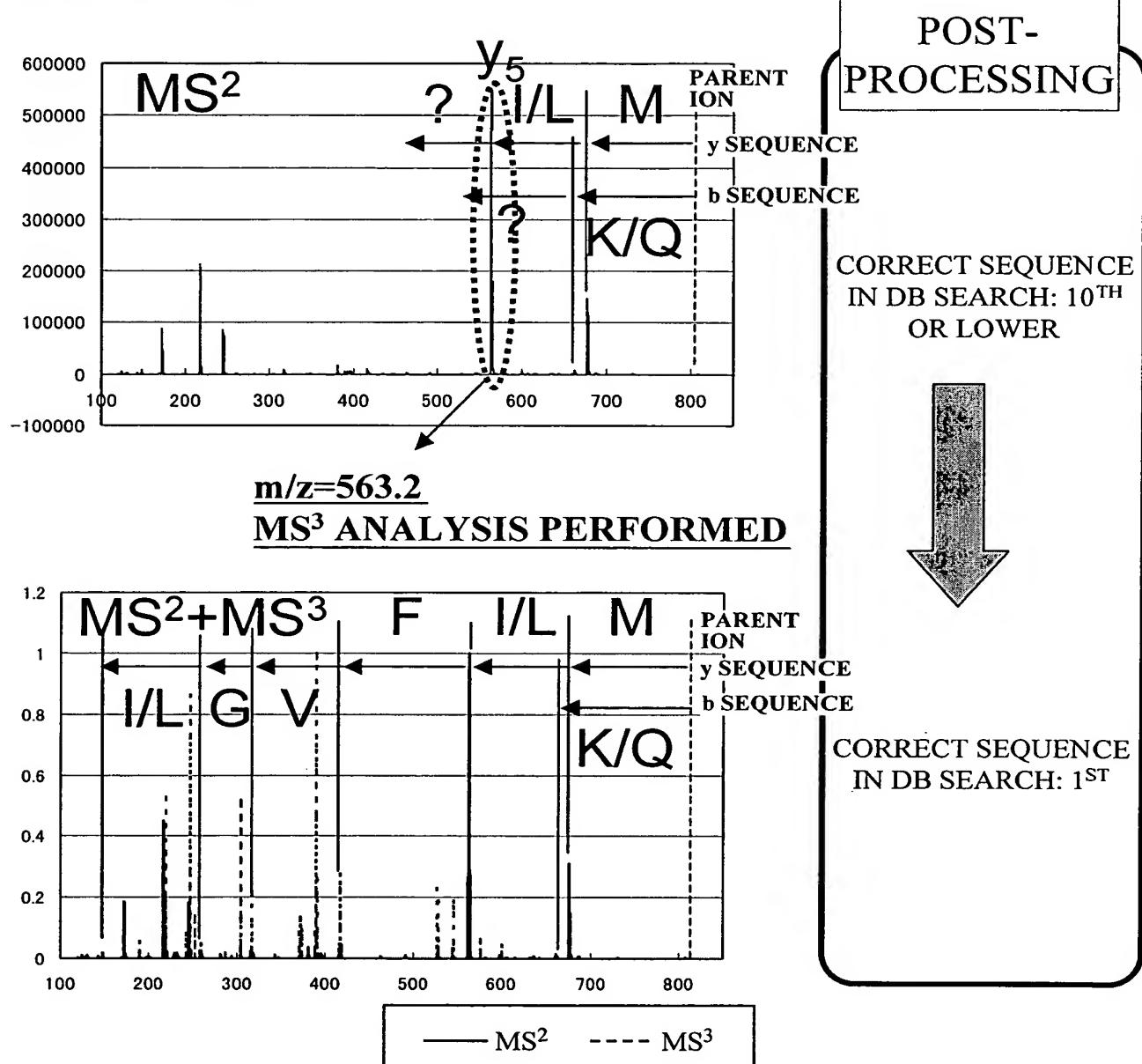


FIG. 38

FLOWCHART (REAL-TIME DB SEARCH)

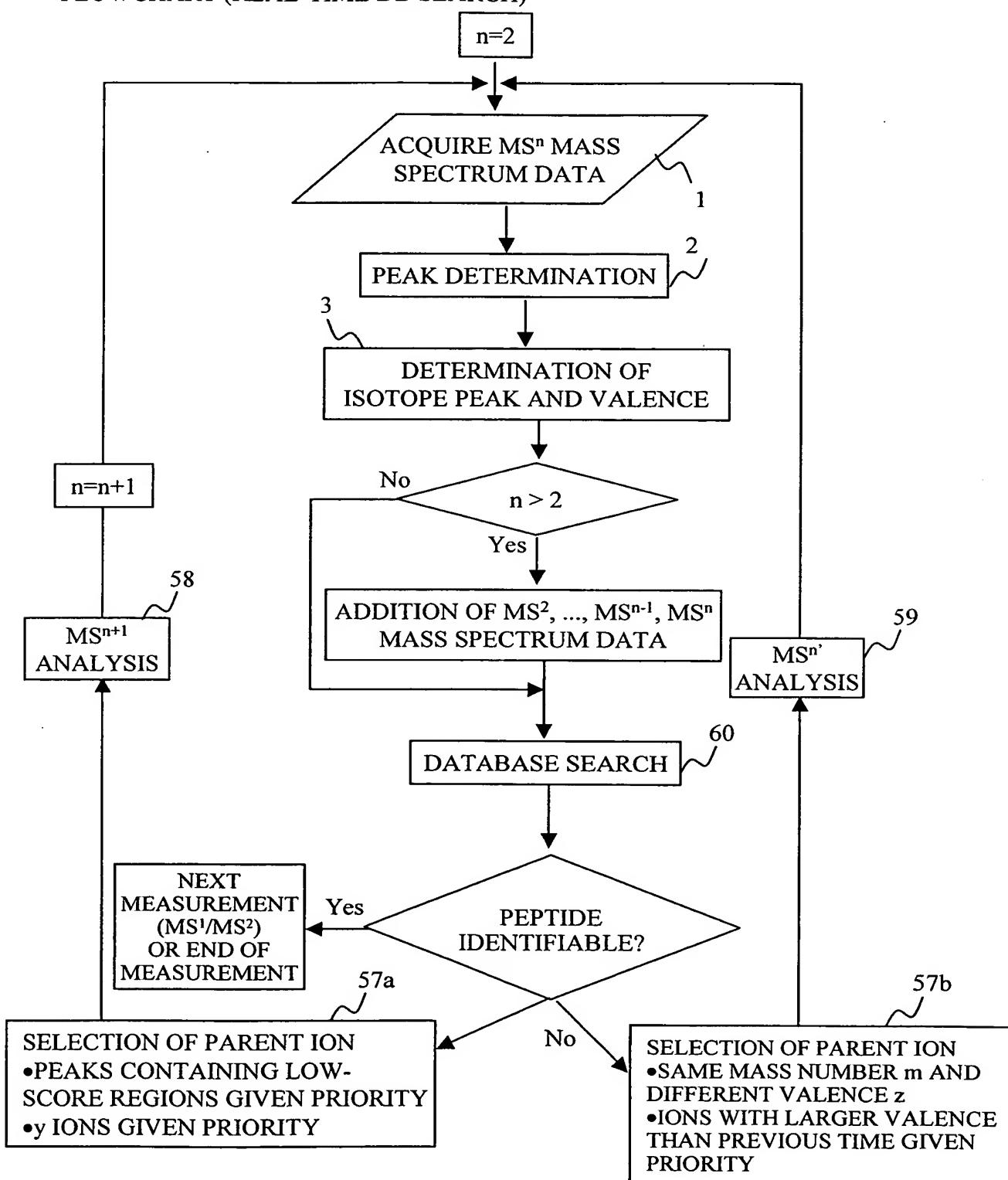


FIG. 39

(FLOWCHAR: SPECIFIC CONDITIONS → MS3/MS2')

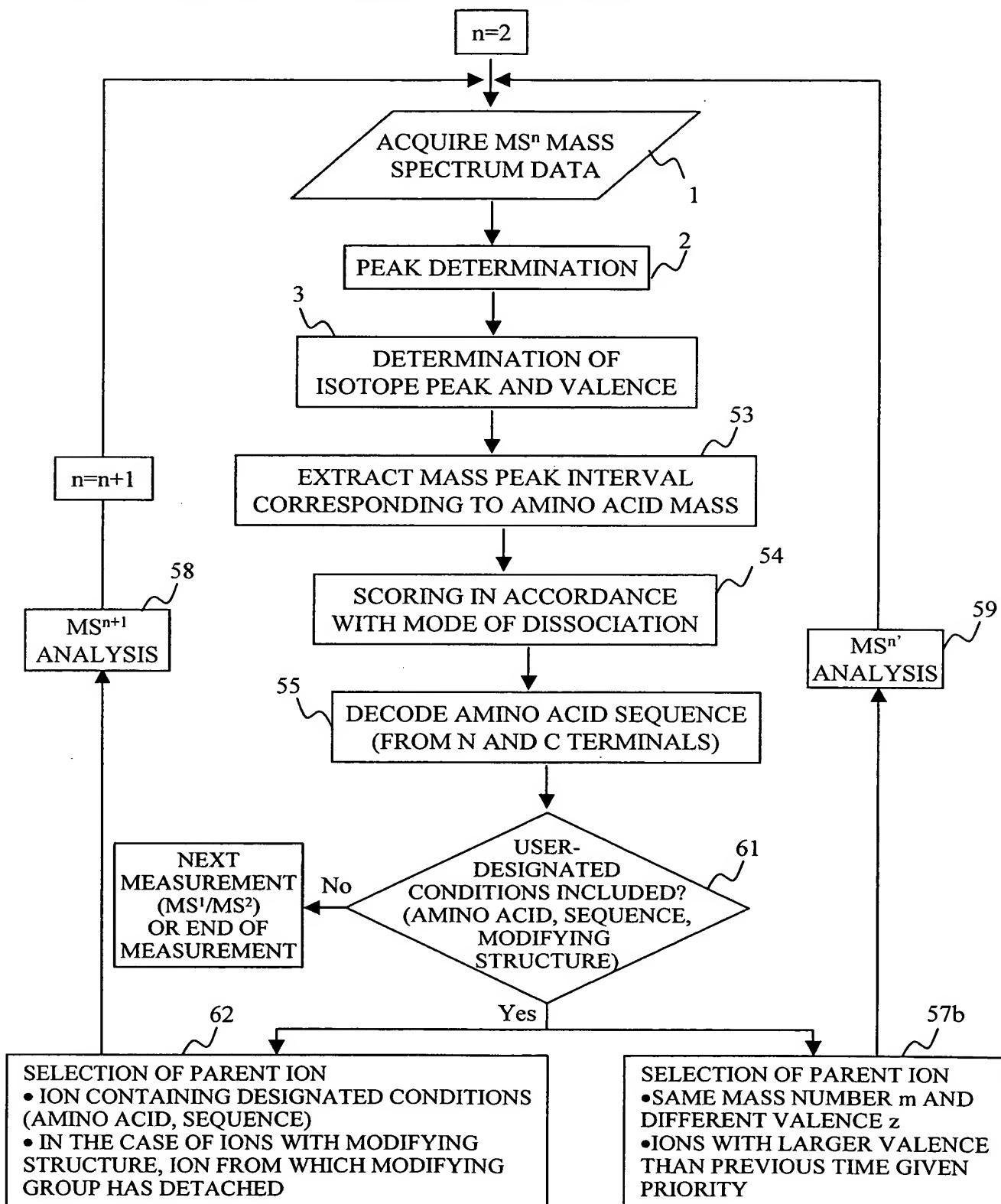


FIG. 40

(DERIVATION OF NUMBER OF PEAK GROUPS)

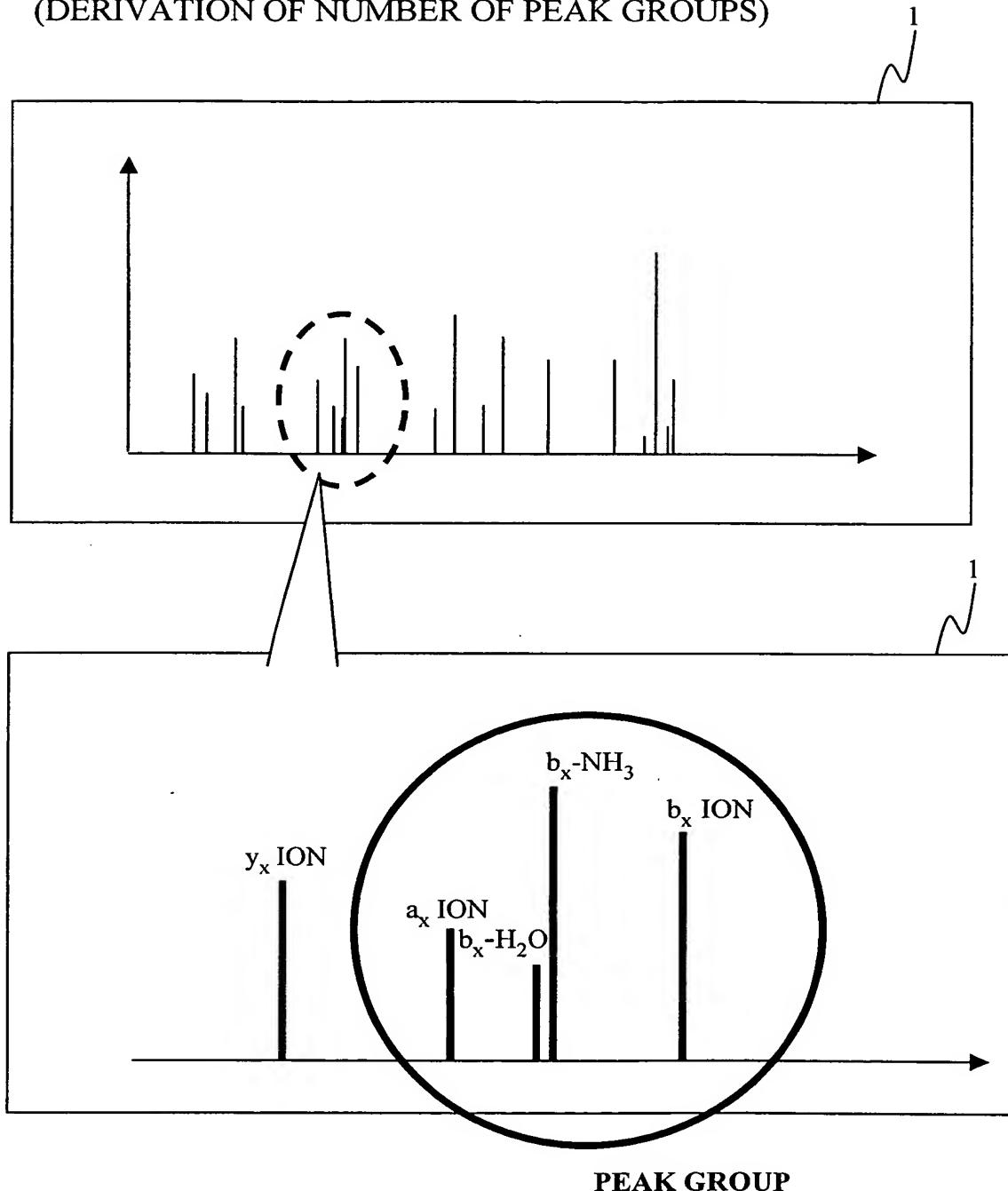


FIG. 41

(FLOWCHART: DETERMINATION BASED ON PEAK GROUP)

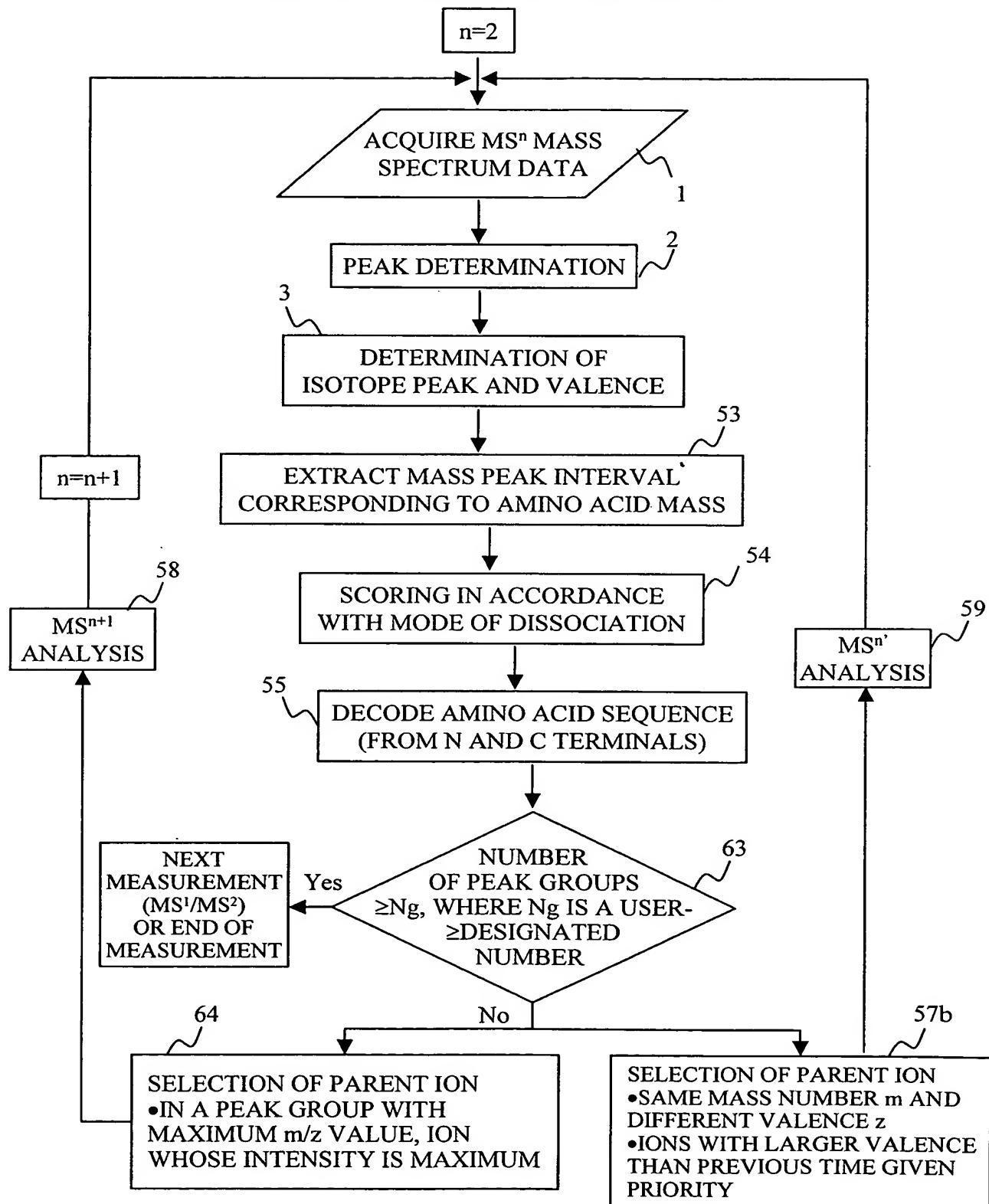


FIG. 42

(FLOWCHART: DETERMINATION BASED ON NUMBER OF PEAKS)

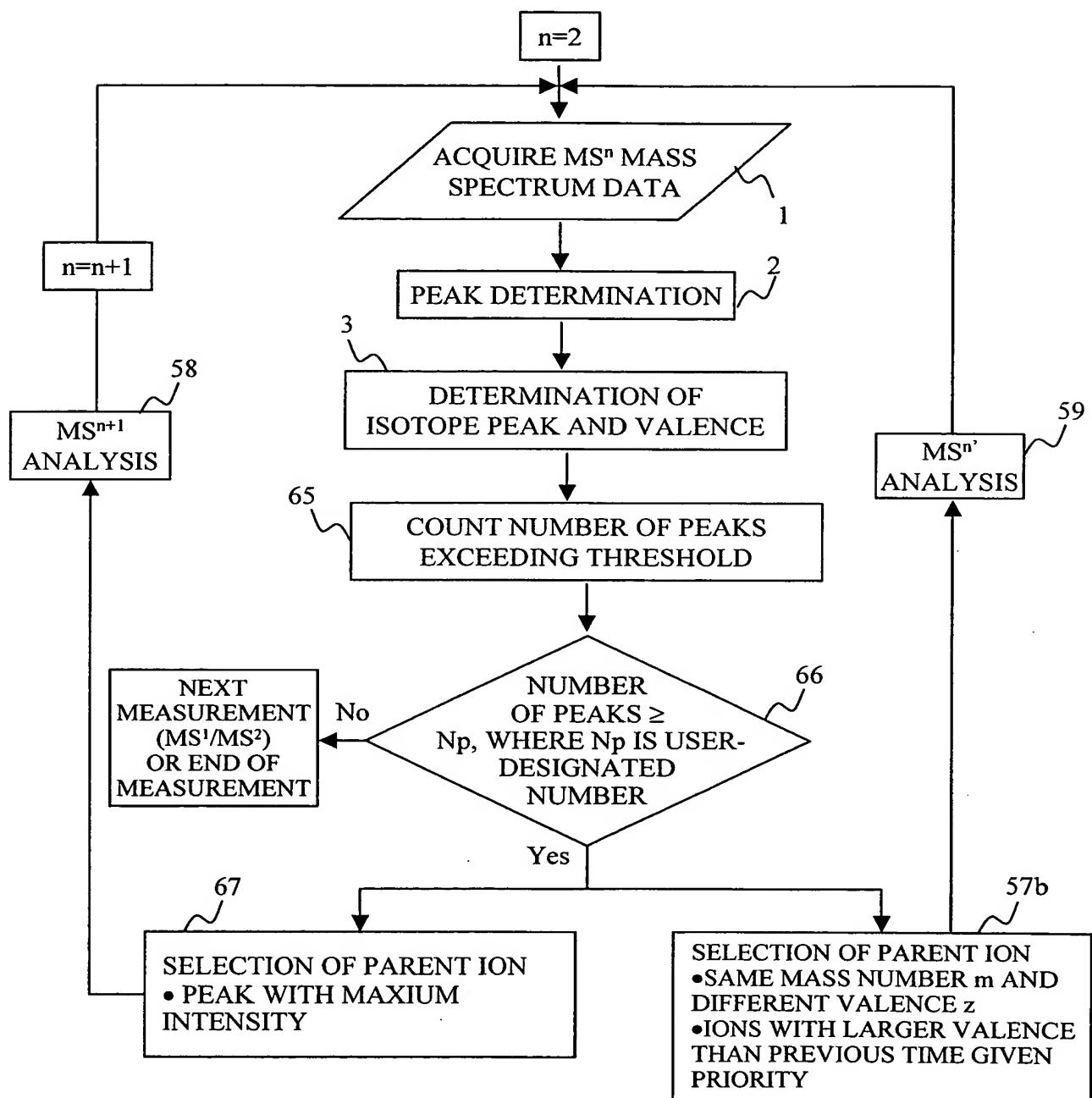


FIG. 43

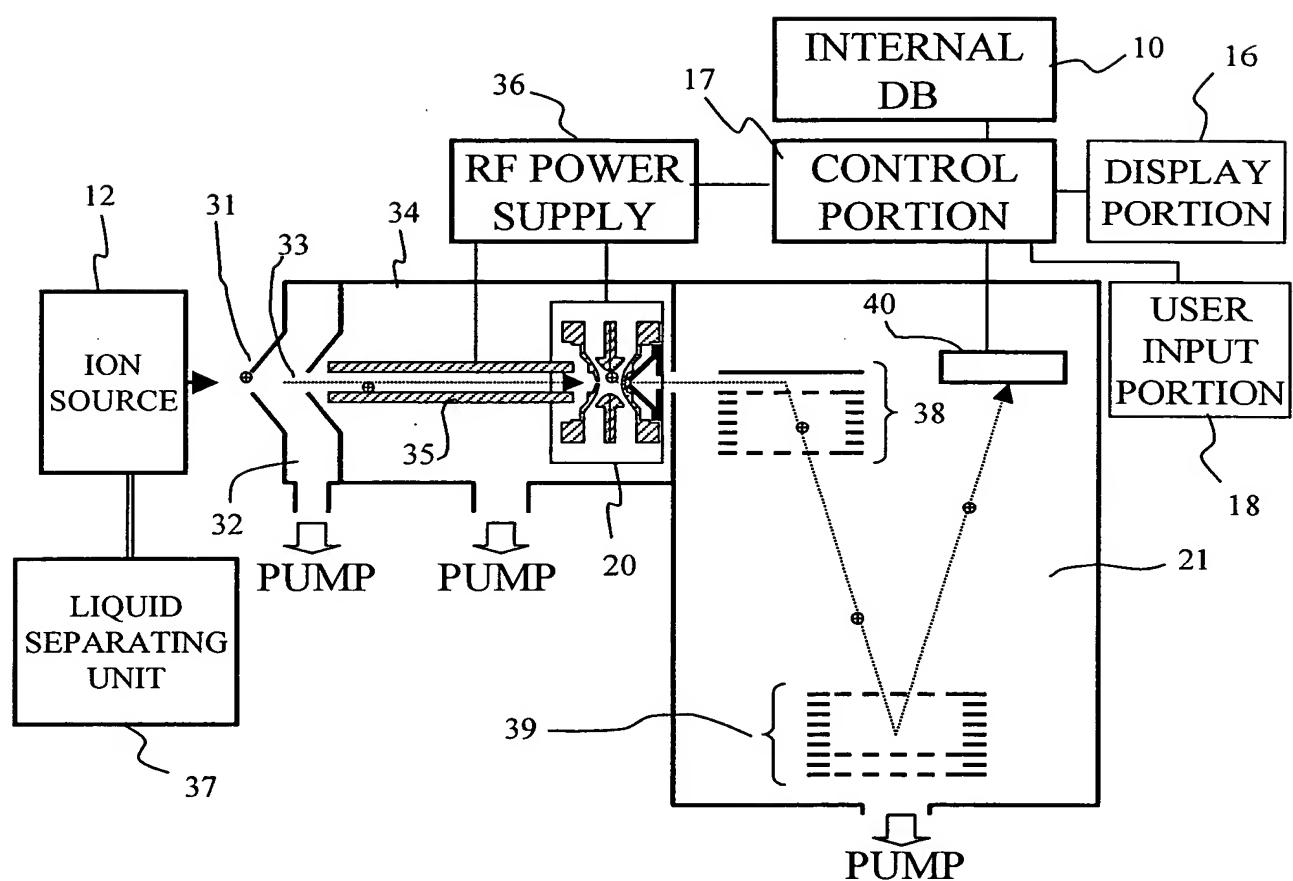


FIG. 44

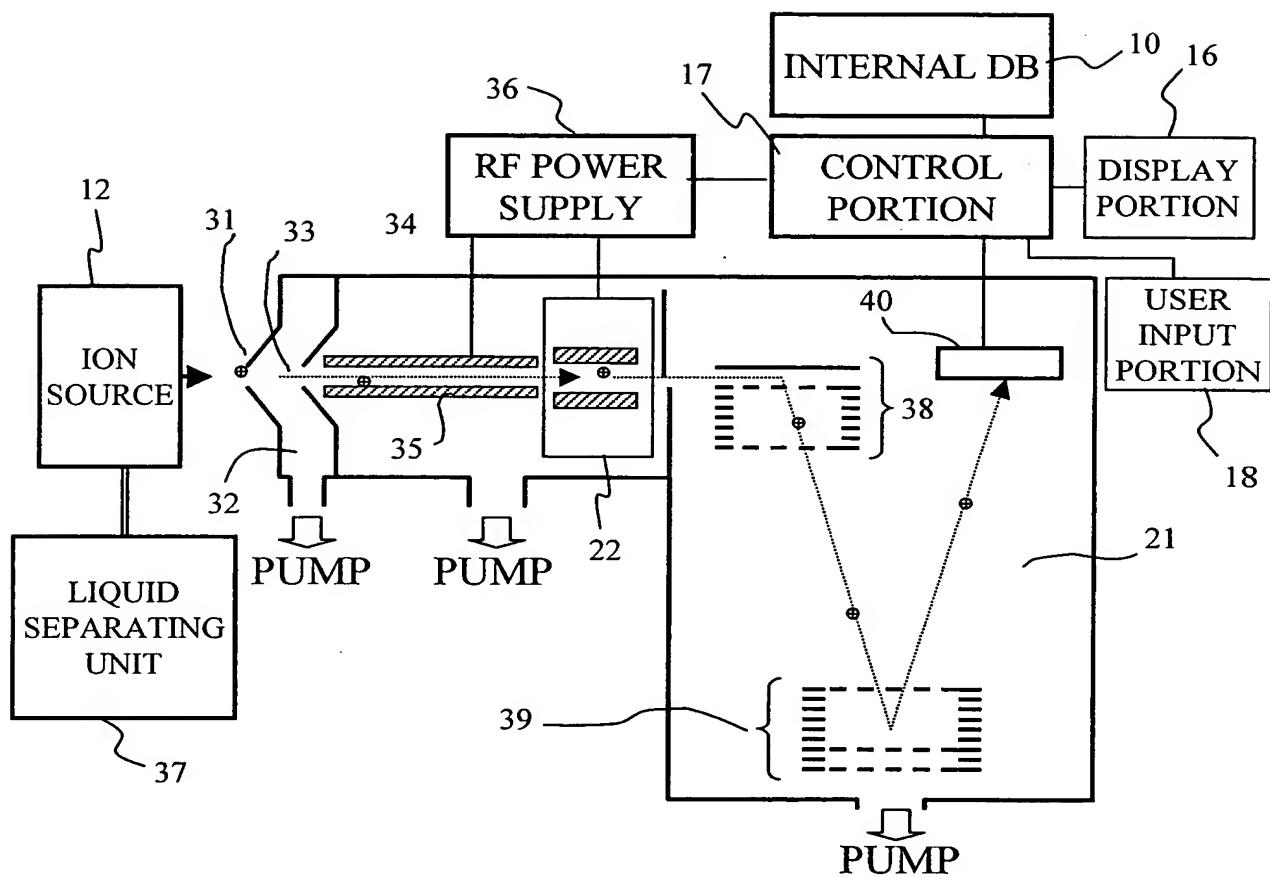


FIG. 45

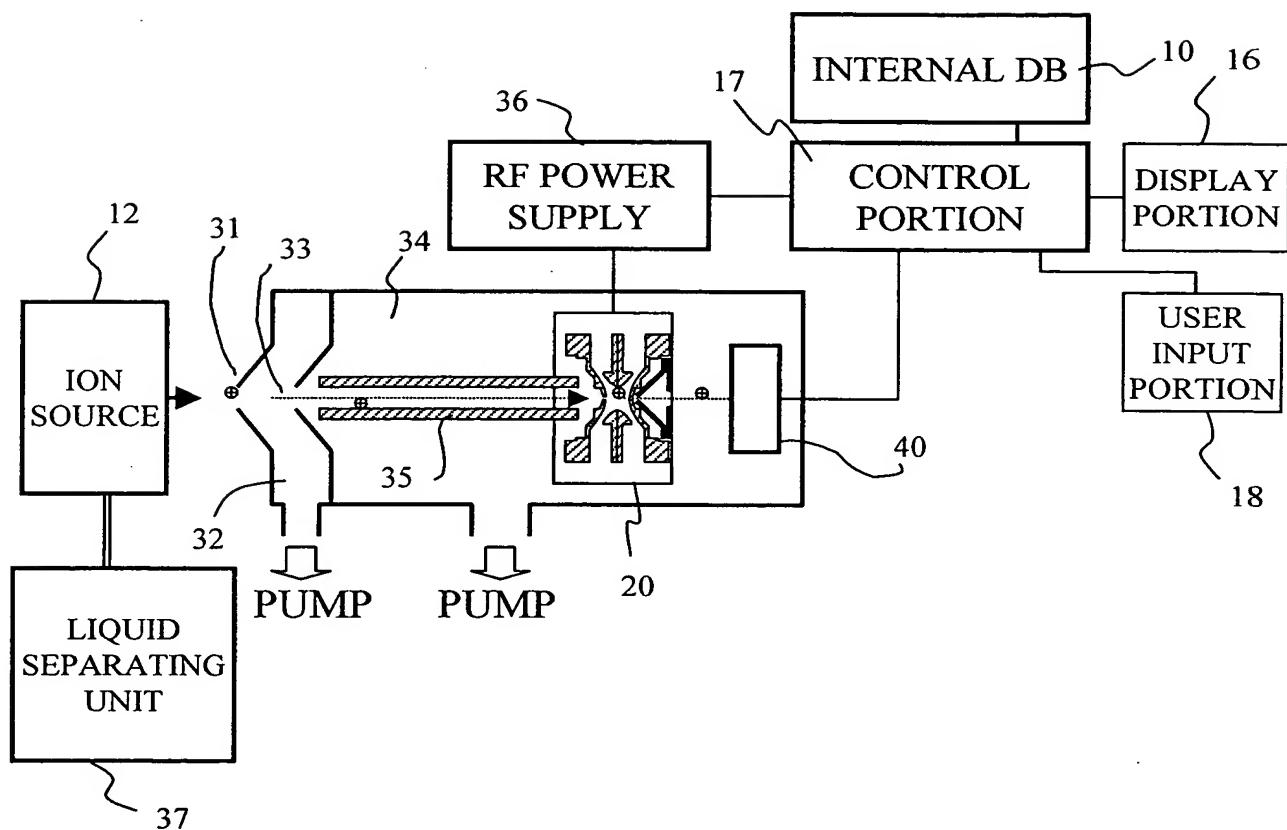


FIG. 46

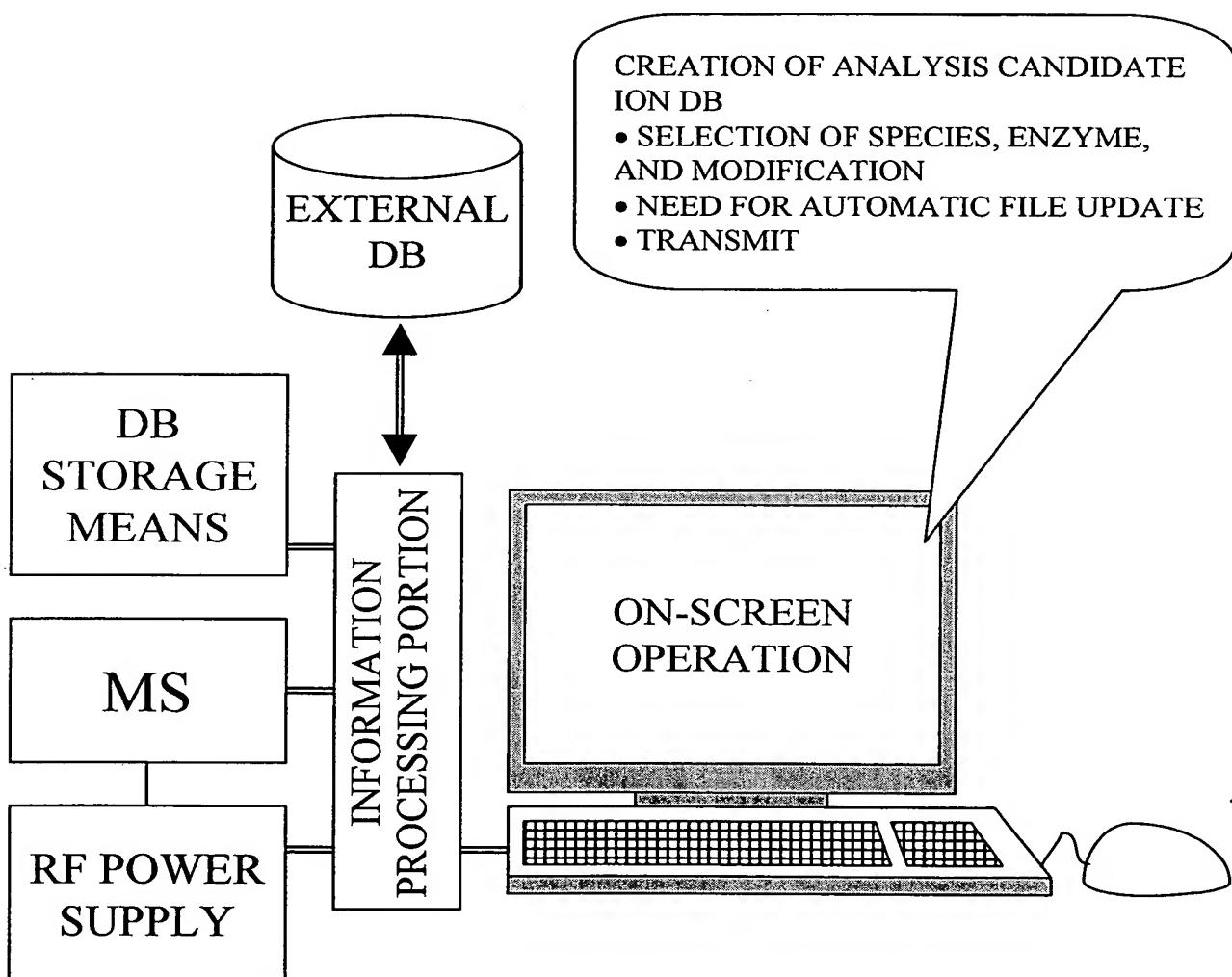


FIG. 47

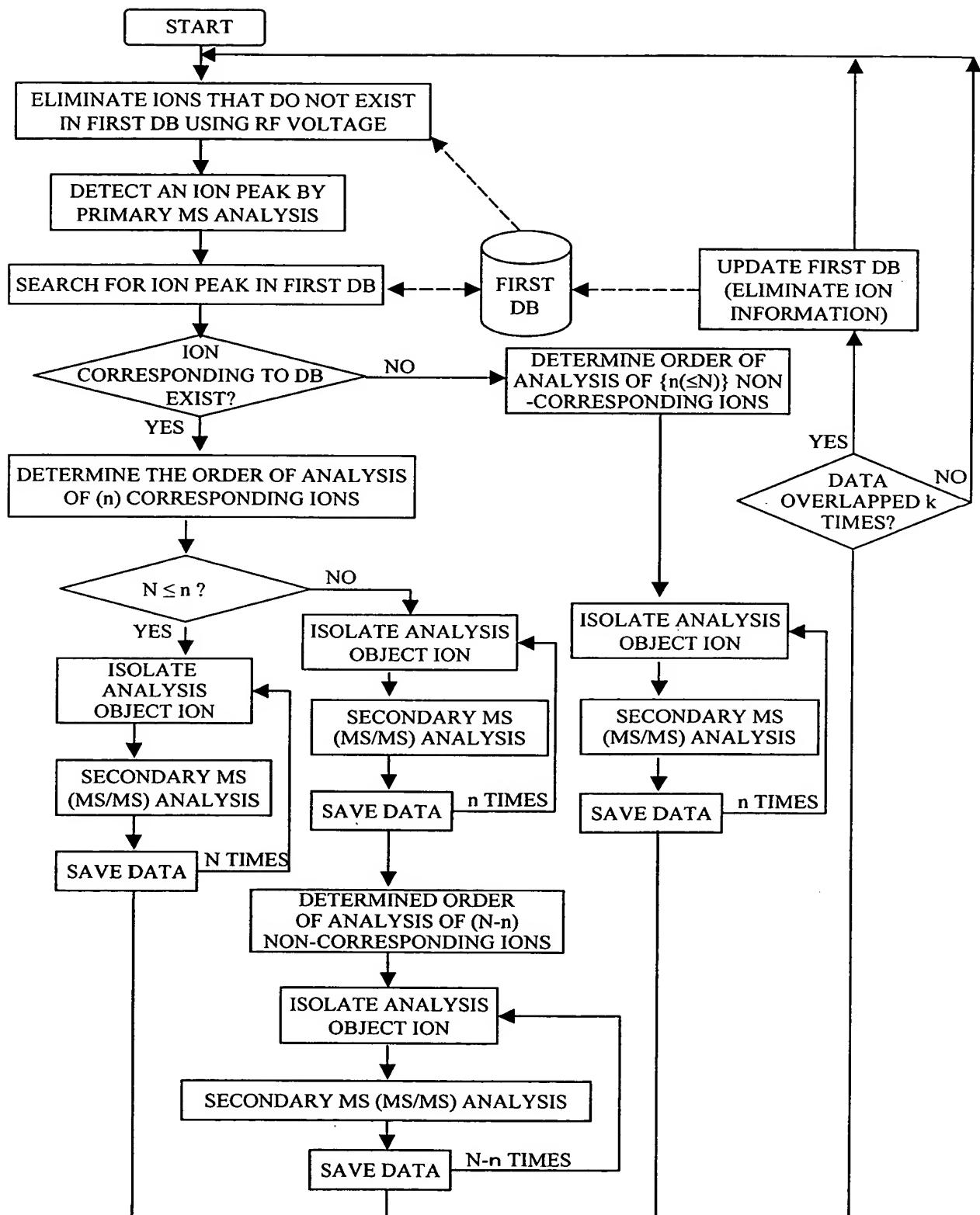


FIG. 48

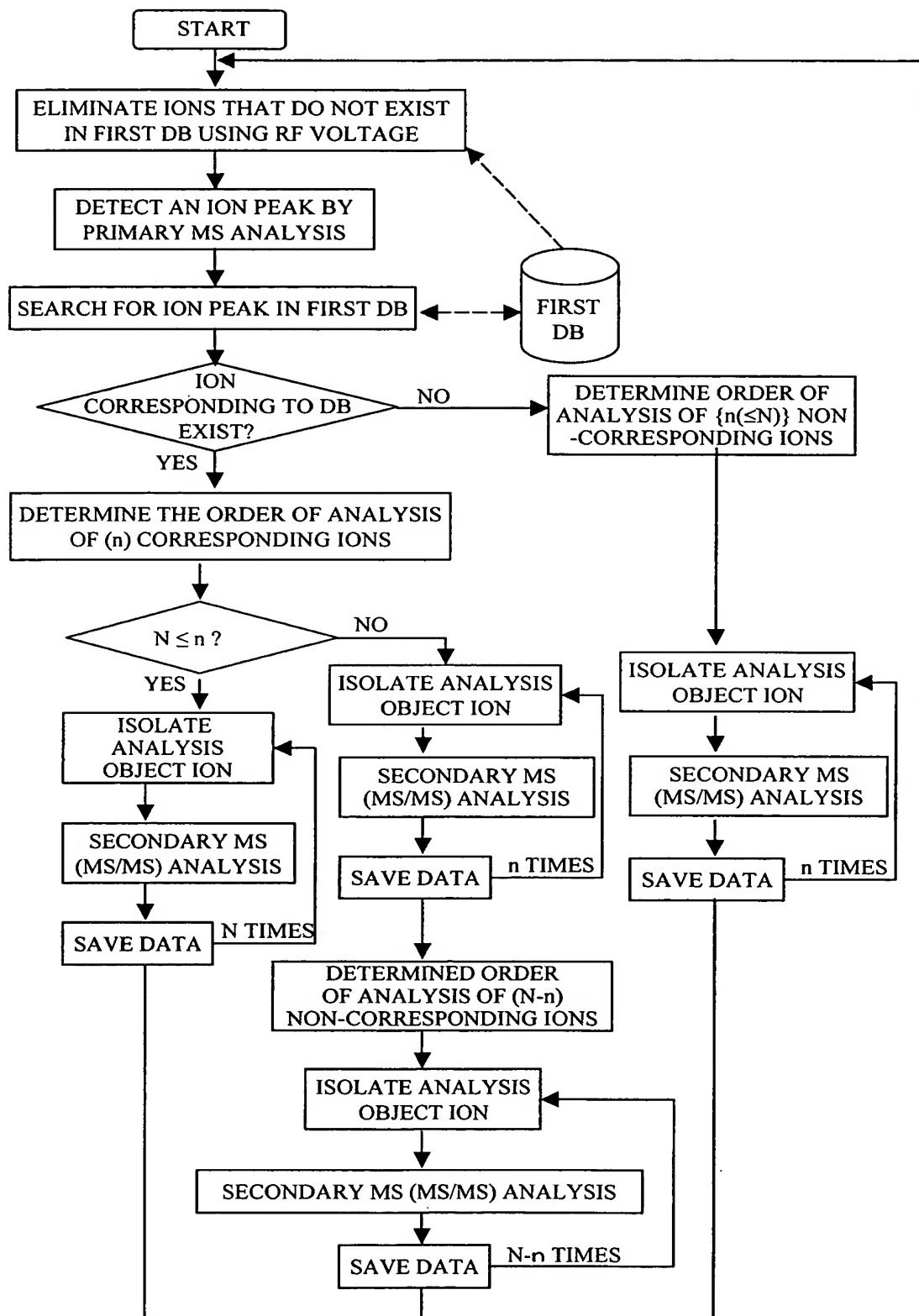


FIG. 49

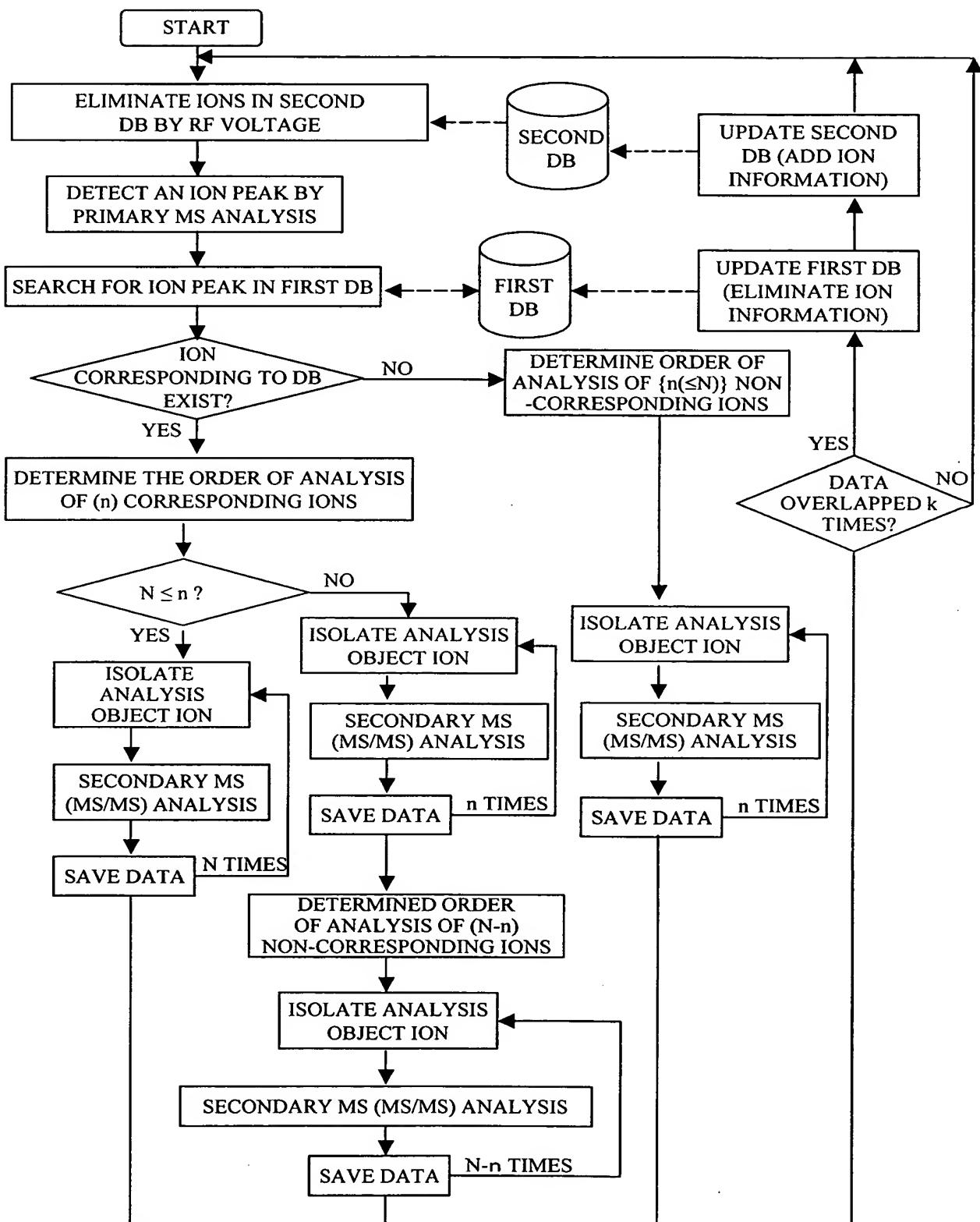


FIG. 50

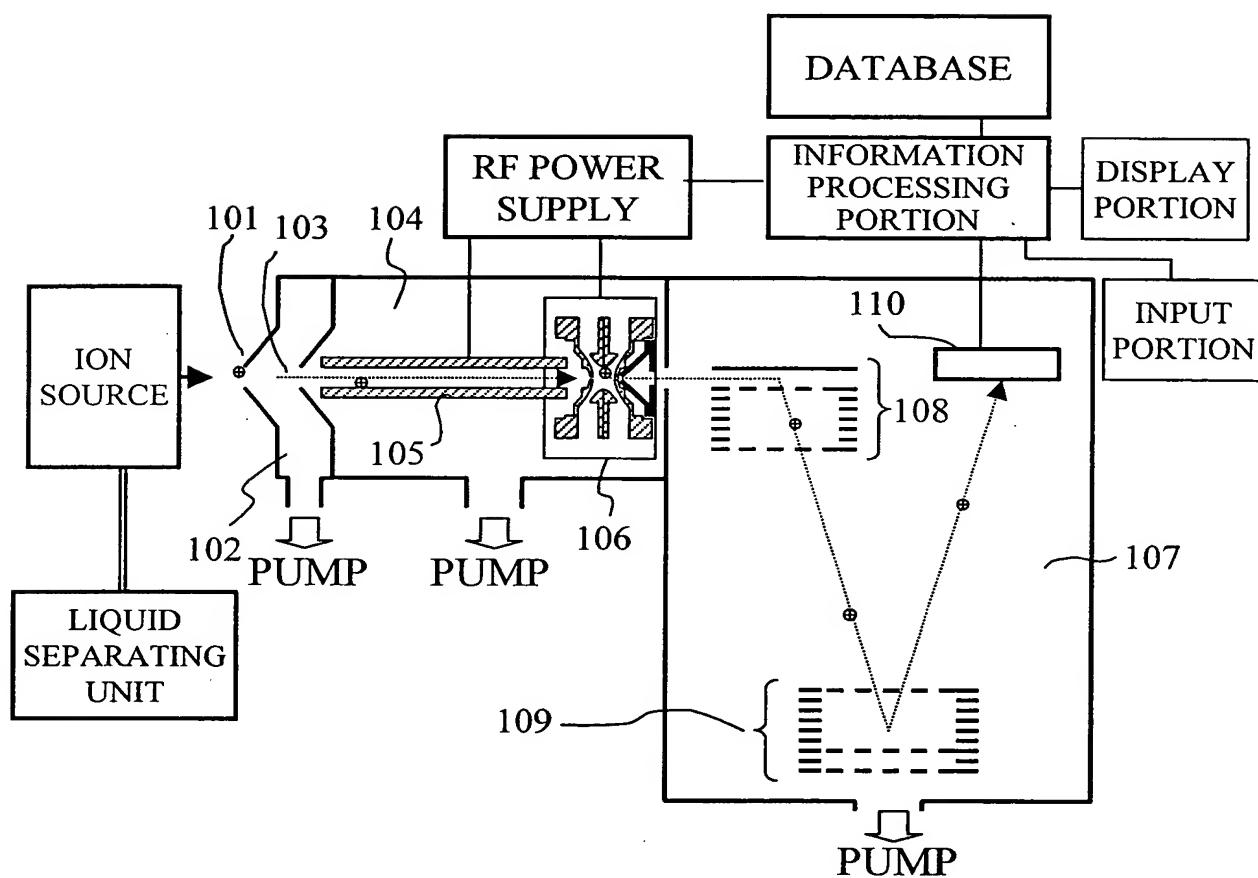


FIG. 51

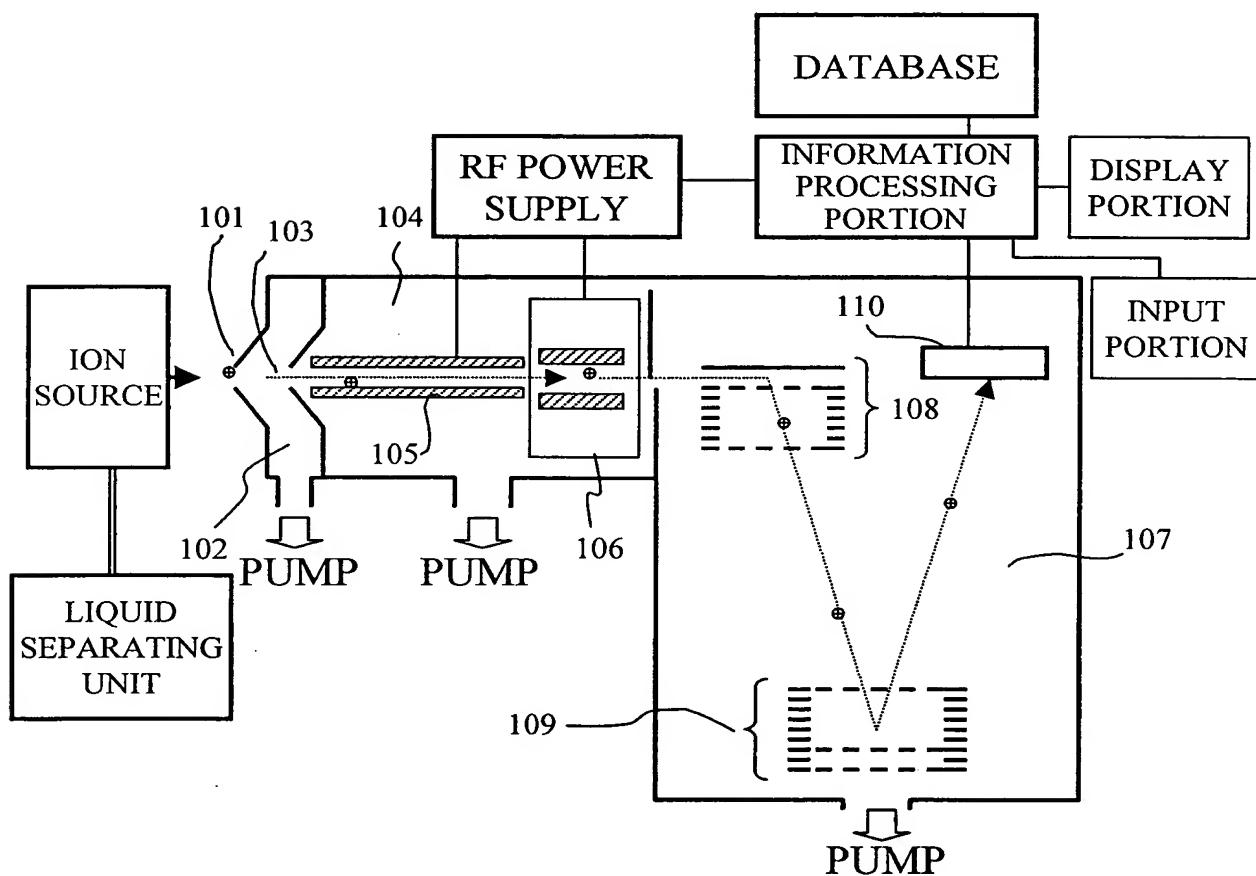


FIG. 52

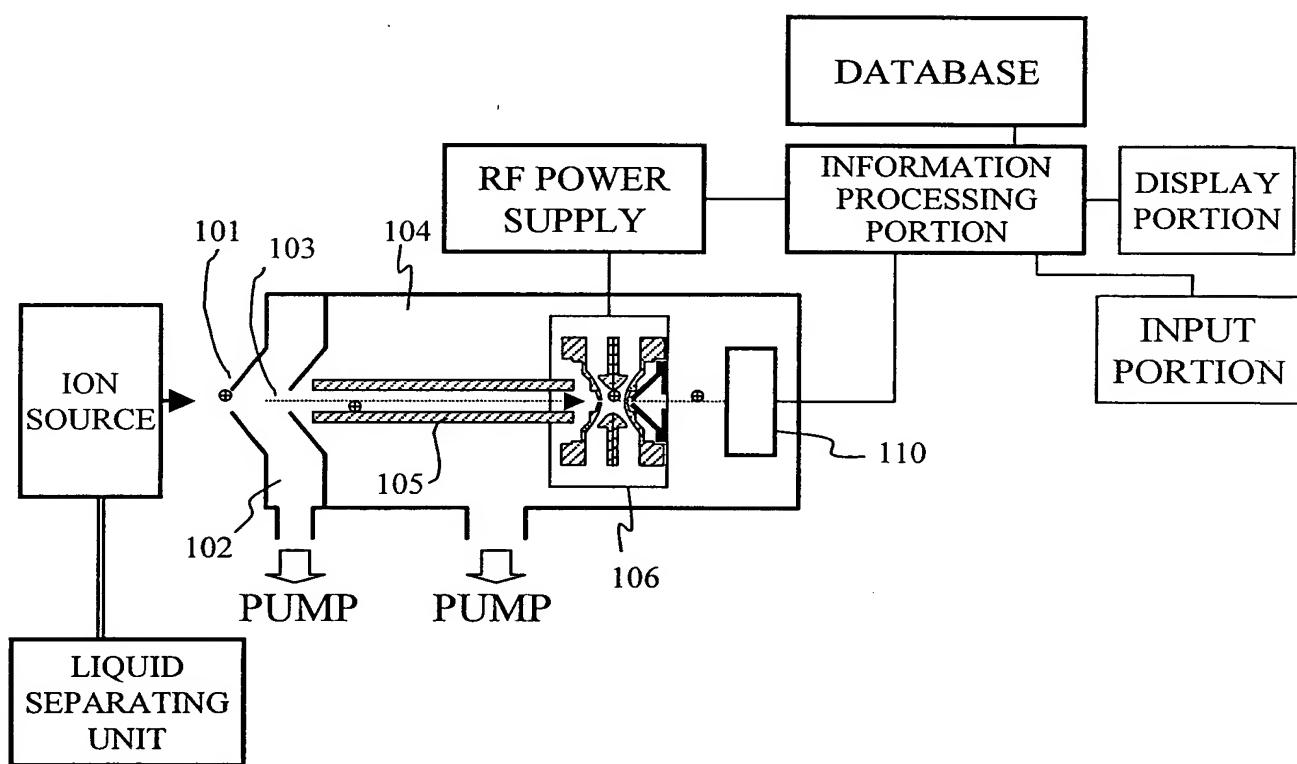


FIG. 53 a

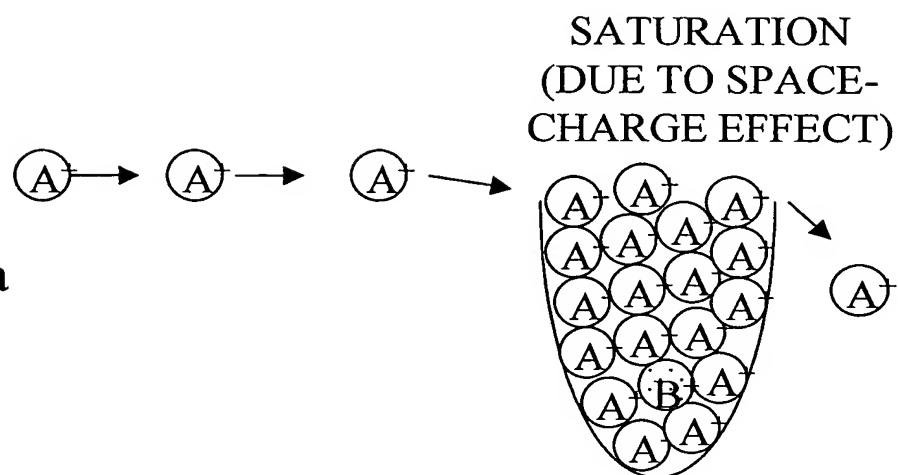
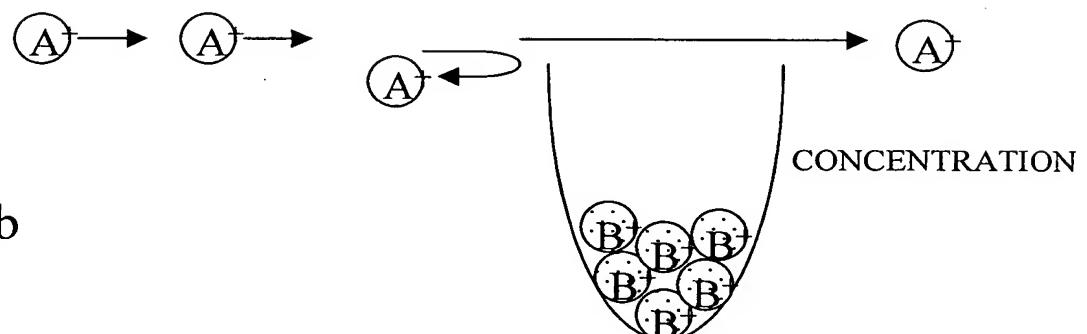


FIG. 53 b



ION TRAP

FIG. 54

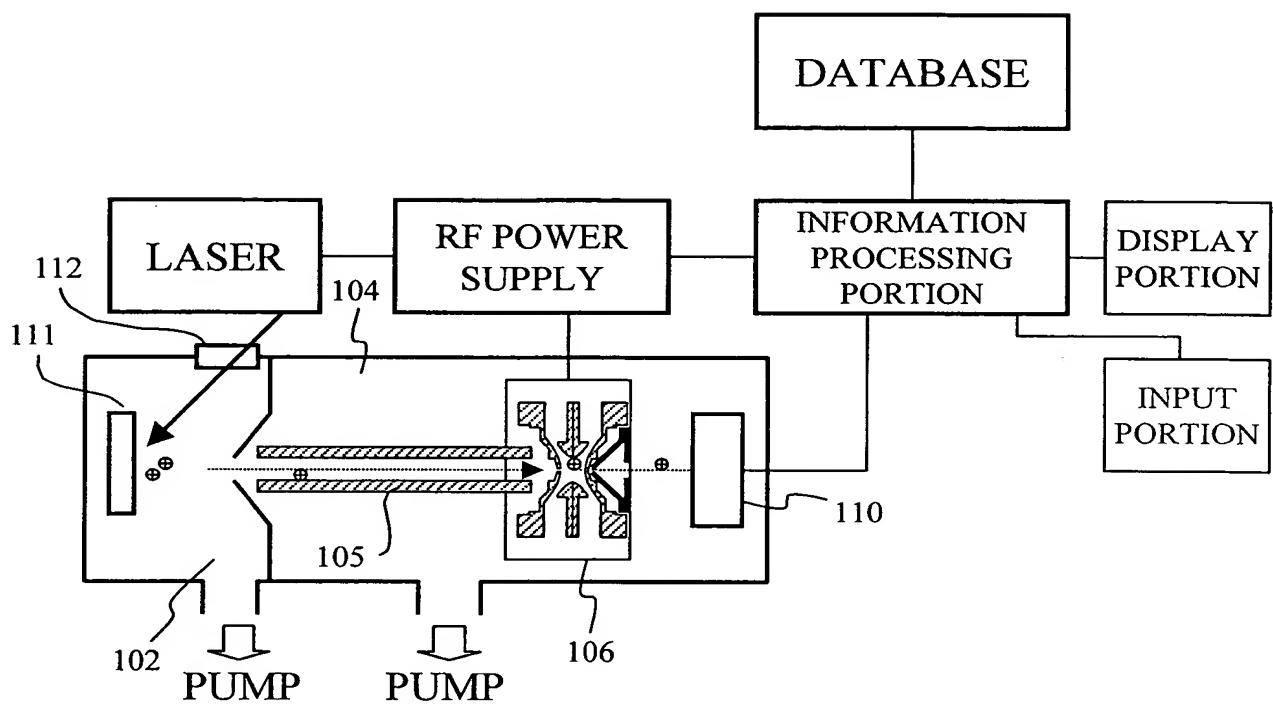


FIG. 55

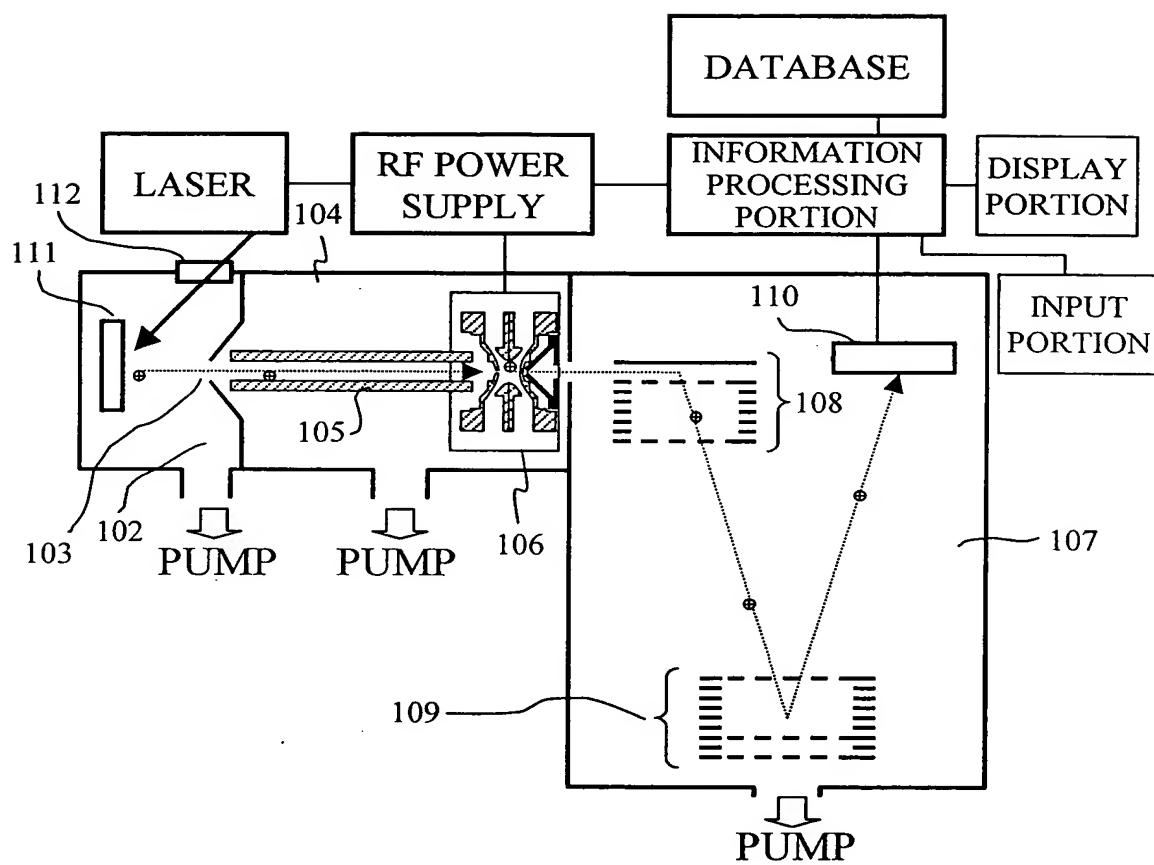


FIG. 56

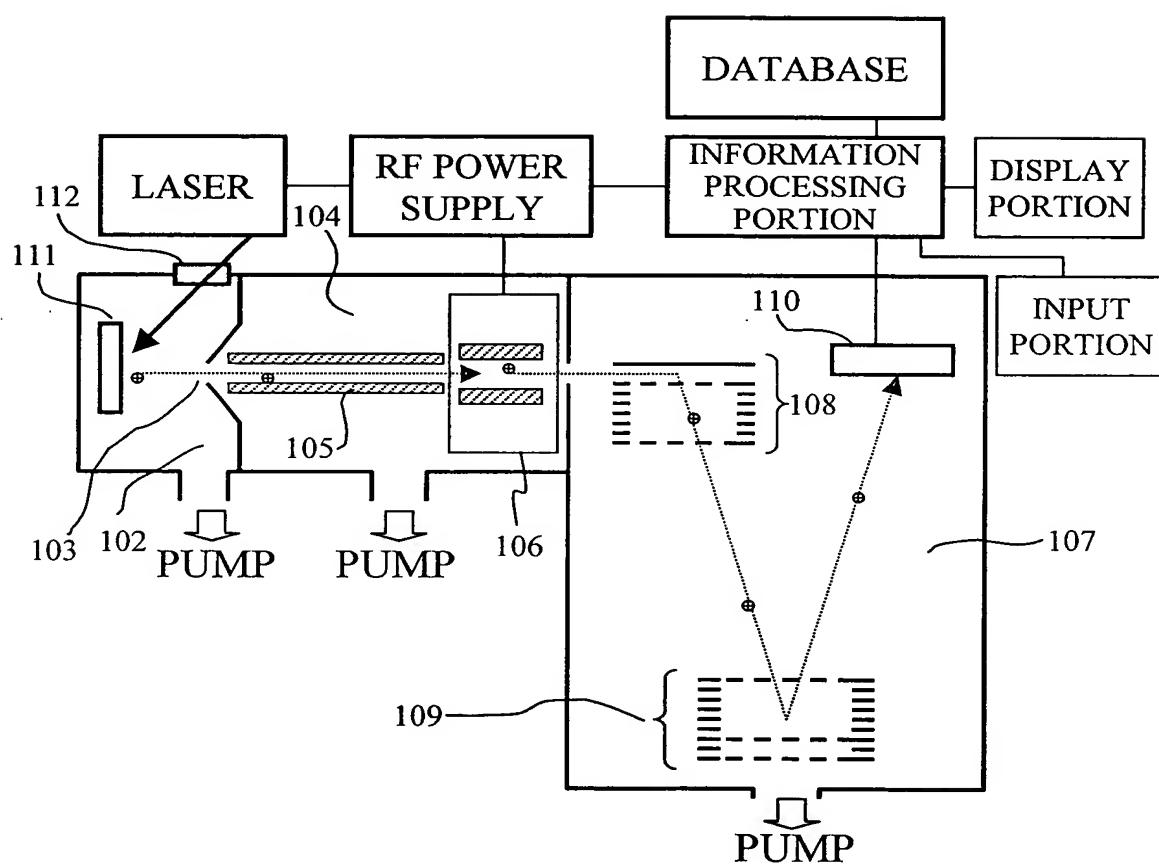


FIG. 57

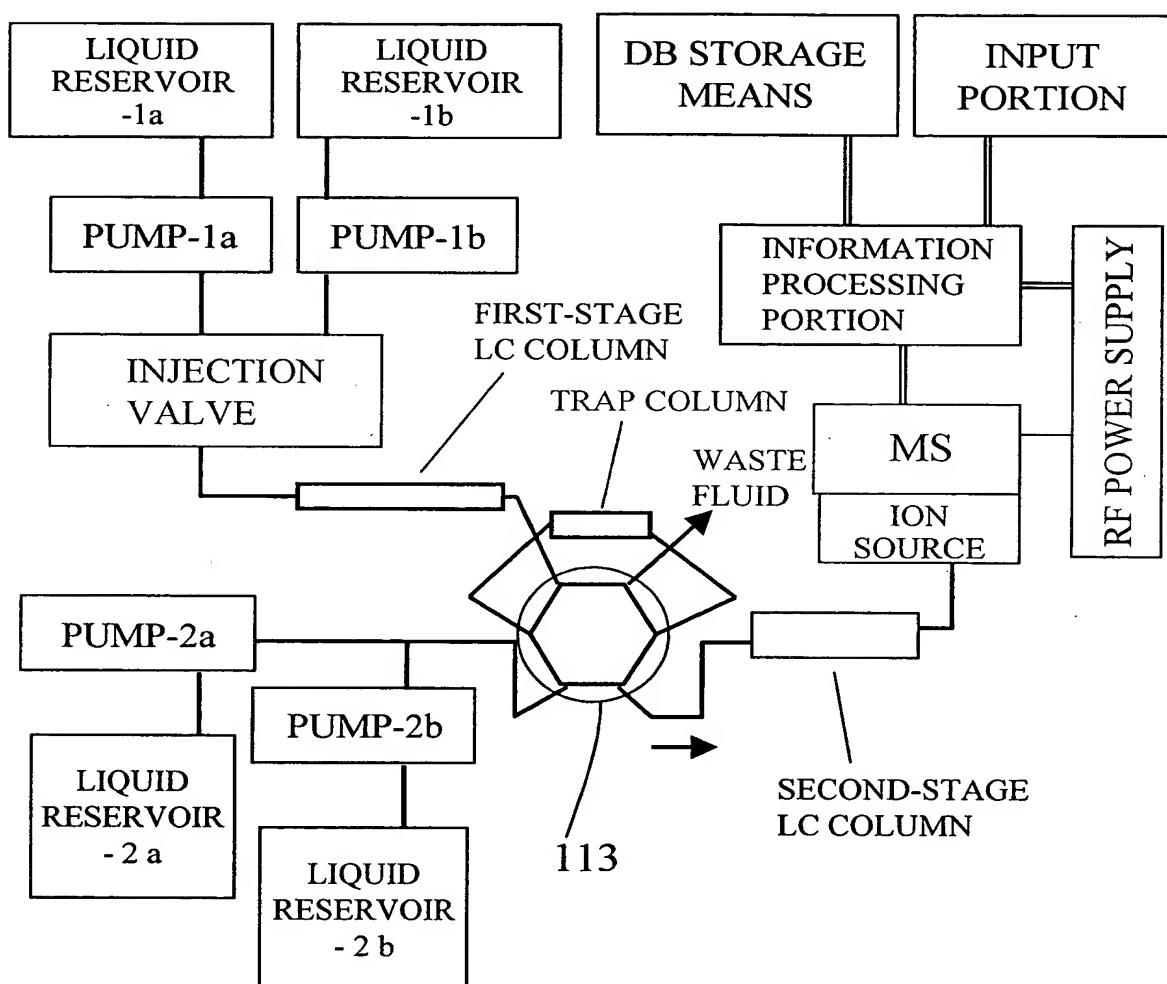


FIG. 58

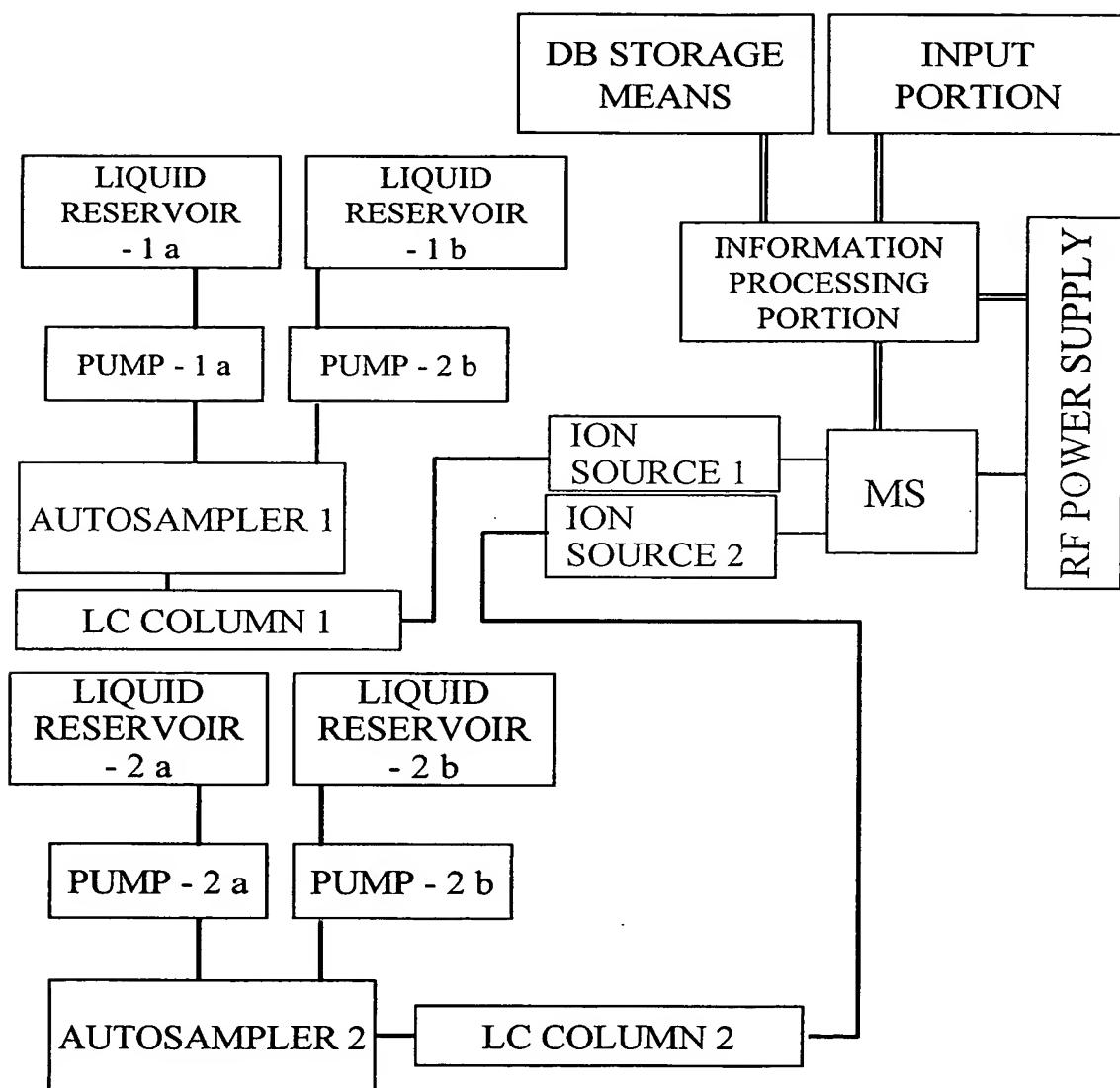


FIG. 59

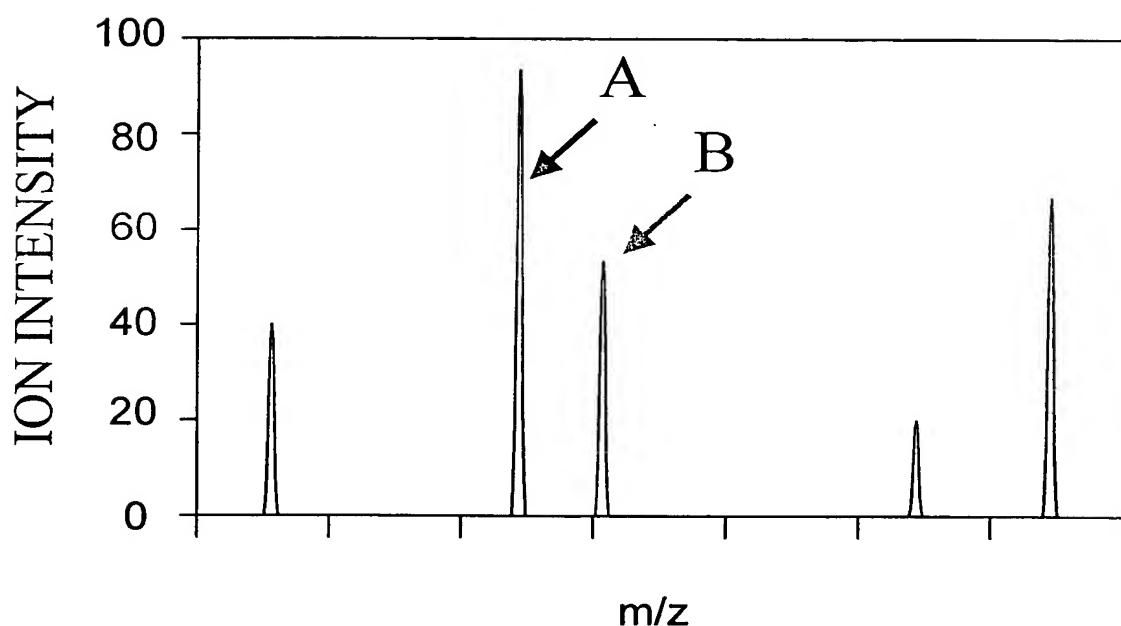
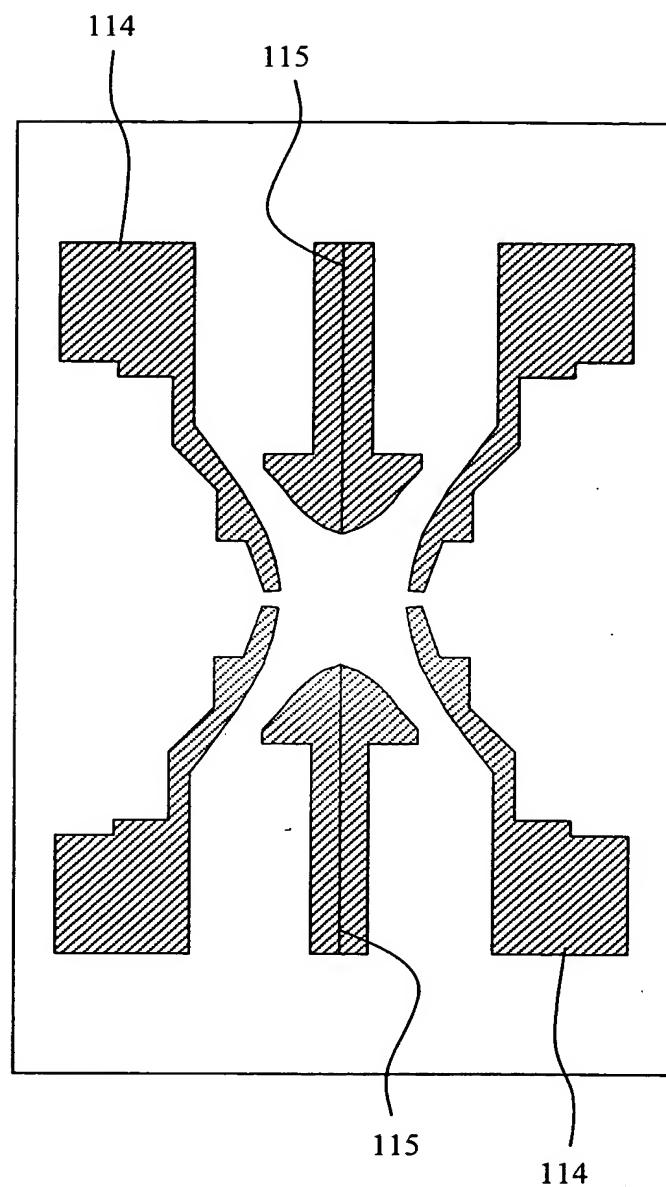


FIG. 60



**This Page is Inserted by IFW Indexing and Scanning
Operations and is not part of the Official Record**

BEST AVAILABLE IMAGES

Defective images within this document are accurate representations of the original documents submitted by the applicant.

Defects in the images include but are not limited to the items checked:

- BLACK BORDERS**
- IMAGE CUT OFF AT TOP, BOTTOM OR SIDES**
- FADED TEXT OR DRAWING**
- BLURRED OR ILLEGIBLE TEXT OR DRAWING**
- SKEWED/SLANTED IMAGES**
- COLOR OR BLACK AND WHITE PHOTOGRAPHS**
- GRAY SCALE DOCUMENTS**
- LINES OR MARKS ON ORIGINAL DOCUMENT**
- REFERENCE(S) OR EXHIBIT(S) SUBMITTED ARE POOR QUALITY**
- OTHER:** _____

IMAGES ARE BEST AVAILABLE COPY.

As rescanning these documents will not correct the image problems checked, please do not report these problems to the IFW Image Problem Mailbox.